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NJUGUNA, J., STAROST, K., VERDEJO, R. (eds.)

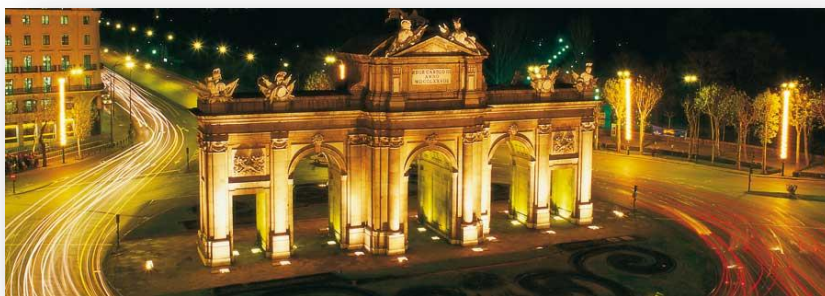
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NANOSTRUC 2014

International Conference on Structural Nano Composites
20-21 May 2014 in Madrid, Spain

Abstract Book



Conference Theme: Nanosciences and Nanotechnologies – Recent Advances towards Nanoproducts and Applications

In conjunction with:



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Preface



Dear Colleagues,

It is a great pleasure to welcome you to NANOSTRUC 2014 at CSIC, Madrid, Spain.

The nanoparticles and nanocomposites have a wide range of applications in various fields such as medicine, textiles, cosmetics, agriculture, optics, food packaging, optoelectronic devices, semiconductor devices, aerospace, automotive, construction and catalysis. Advancements in the nanotechnology industry promise to offer improvements in capabilities across a spectrum of applications. This is of immense strategic importance to the high performance sector which has historically leveraged technological advances in materials.

The purpose of The 2nd International Conference on Structural Nano Composites (NANOSTRUC 2014) is to promote activities in various areas of materials and structures by providing a forum for exchange of ideas, presentation of technical achievements and discussion of future directions. NANOSTRUC brings together an international community of experts to discuss the state-of-the-art, new research results, perspectives of future developments, and innovative applications relevant to structural materials, engineering structures, nanocomposites, modelling and simulations, and their related application areas. We would like to acknowledge the hard work, professional skills and efficiency of the team which ensured the general organisation.

We would like to Welcome you to the NANOSTRUC 2014 and wish you a stimulating Conference and a wonderful time.

We look forward to meet and welcome you at Madrid.

Yours sincerely,

A handwritten signature in blue ink, appearing to read 'James Njuguna'.

A handwritten signature in blue ink, appearing to read 'R. Verdejo'.

James Njuguna & Raquel Verdejo

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High temperature applications - Kanda Balasubramanian - *Defense Institute of Advanced Technology, India*
Water Applications - Ajay Mishra - *University of Johannesburg, South Africa*
Biocomposites and nanofibres - Susheel Kalia - *University of Bologna, Italy*
Nanopigment and Colorants - Veronica Marchante - *Cranfield University, UK*
Safety of nanomaterials throughout their life cycle - Maria Blazquez - *Inkoa, Spain*
Life Cycle Analysis and Technological Assessment (TBC) - Marcel Weil - *Karlsruhe Institute of Technology, Germany & Claudia Som, EMPA, Switzerland*
Poster session - Sponsored by WILEY-VCH Verlag GmbH & Co. KGaA, and Nanotechnology Industries Association (NIA)
First International Workshop of the SIRENA-Life Project - Maria Blazquez - *Inkoa, Spain*

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Programme at a Glance

Monday 19th May 2014

Time	Programme point
16:00-19:00	Pre-Registration + Drinks Reception

Nanostruc Day 1 - Tuesday 20th May 2014

Time	Programme point
07:30 - 9:00	REGISTRATION
08:30	Welcome and Introductions
09:00-13:00	Morning Parallel Sessions
09:00 - 10:30	Session 1.1: Application of Nanomaterials and Nanocomposites - Dan Batalu Session 2.1: Graphene and Carbon-based Nanocomposites - Jinbo Bai Session 3.1: Functional Nanocomposites - Ajay Mishra
10:30 - 11:00	<i>Coffee Break</i>
11:00 - 13:00	Session 1.2: Application of Nanomaterials and Nanocomposites (Automotive and Aerospace) Session 2.2: Graphene and Carbon-based Nanocomposites -Sami Boufi Session 3.2: Functional Nanocomposites - Krzysztof Pielichowski
13:00 -14:00	<i>Lunch Break</i>
14:00-18:00	Afternoon Parallel Sessions
14:00-15:40	Session 1.3: Application of Nanomaterials and Nanocomposites (Performance) Session 2.3: Graphene and Carbon-based Nanocomposites - Eduardo Ruiz-Hitzky Session 3.3: Functional Nanocomposites & Nanopigments/Colorants - Veronica Marchante
15:30-16:00	<i>Coffee Break</i>
16:00-18:00	Session 1.4: Application of Nanomaterials and Nanocomposites (Performance) - Fawad Inam Session 2.4: Biocomposites and Nanofibres - Susheel Kalia Session 3.4: Water Applications
18:00 - 19:30	Poster Session - Sponsored by WILEY-VCH Verlag GmbH & Co. KGaA, and Nanotechnology Industries Association (NIA)
20:30	Gala Dinner

Nanostruc Day 2 - Wednesday 21st May 2014

Time	Programme point
9:00 -13:00	Morning Parallel Sessions
	Session 1.5: Application of Nanomaterials and Nanocomposites (Sensory Materials)
09:00 - 10:30	Session 2.5: Modelling and Simulations
	Session 3.5: FIRST INTERNATIONAL WORKSHOP OF THE SIRENA-LIFE PROJECT - Maria Blasquez
10:30 -11:00	<i>Coffee Break</i>
	Session 1.6: Application of Nanomaterials and Nanocomposites (Coatings)
11:00 - 13:00	Session 2.6: Biomaterials and Biomedical devices
	Session 3.6: FIRST INTERNATIONAL WORKSHOP OF THE SIRENA-LIFE PROJECT - Maria Blasquez
13:00 -14:00	<i>Lunch Break</i>
14:00-18:00	Afternoon Parallel Sessions
14:00-15:40	Session 1.7: Application of Nanomaterials and Nanocomposites (Thin Films) - Veronicah Marchante
	Session 2.7: Biomaterials and Biomedical devices (Antibacterial)
	Session 3.7: Life Cycle Analysis (LCA) and Constructive Technology Assessment (CTA) for Nano-Enabled Technologies - Marcel Weil & Claudia Som
15:30-16:00	<i>Coffee Break</i>
	Session 1.8: Application of Nanomaterials and Nanocomposites (Thin Films)
16:00-18:00	Session 2.8: Biomaterials and Biomedical devices (Antibacterial)
	Session 3.8: Life Cycle Analysis (LCA) & Constructive Technology Assessment (CTA) for Nano-Enabled Technologies - Marcel Weil & Claudia Som
18:00	EVENT CLOSSURE

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Fibrous Clays-based Bionanocomposites

Eduardo Ruiz-Hitzky*

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This lecture will introduce the latest progresses in the preparation of bionanocomposites based on fibrous clays such as sepiolite and palygorskite, assembled to biopolymers of different nature (polysaccharides, proteins and nucleic acids). Both clays are natural microfibrillar silicates whose particular structural, morphological and textural features have opened the way for the preparation of a wide variety of advanced nanostructured bio-hybrid materials¹ including bionanocomposites of interest as structural and functional materials².

Sepiolite, and in minor extent palygorskite, included into diverse biopolymer matrices conferred interesting properties to the resulting nanocomposites offering a wide range of potential applications such as insulating fire-resistant foams, bioplastics with improving barrier properties, new nanostructured materials of interest as drug delivery systems (DDS), and others³. Adsorption of heavy metal ions and other pollutants from waste water by these bionanocomposites show their significance in environmental remediation⁴. DNA non-viral transfection can be reached with sepiolite-DNA bionanocomposites. Finally, biopolymer modified sepiolite can be efficiently used as support of viruses with application as adjuvant of vaccines. Interestingly, the bionanocomposites can be conformed as microparticulated materials (powders), beads, films and foams⁵ showing in some cases a significant enhancement of the mechanical properties in the final materials with respect to the pristine components, which could be related to the nano-structured arrangement and the interfacial interactions between the fibrous inorganic filler and the polymeric counterpart.

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¹ . E. Ruiz-Hitzky, K. Ariga, and Y. Lvov (Eds.). Bio-inorganic Hybrid Nanomaterials: Strategies, Syntheses, Characterization and Applications, Wiley-VCH, Weinheim (2007)

² E. Ruiz-Hitzky, M. Darder, F. M. Fernandes, B. Wicklein, A. C. S. Alcântara, P. Aranda, Prog. Polym. Sci. 38, 1392-1414 (2013)

³ E. Ruiz-Hitzky, M. Darder, P. Aranda, K. Ariga, Adv. Mater. 22, 323-336 (2010)

⁴ E. Ruiz-Hitzky, P. Aranda, M. Darder, M. Ogawa, Chem. Soc. Rev. 40, 801-828 (2011)

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Structural health assessing capabilities in polymeric and ceramic nanocomposites filled with carbon nanofillers

Fawad Inam^{*}

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Carbon nanotubes (CNTs) and graphene are being widely investigated for their addition in polymer, ceramic and metal matrices to prepare nanocomposites owing to the combination of the superlative mechanical, thermal, and electronic properties attributed to them. These materials are subject of significant research interest for their utilisation in an increasing number of applications including energy, transportation, defence, automotive, aerospace, sporting goods, and infrastructure sectors. Particularly among brittle materials (polymers and ceramics), carbon nanofillers have been reported to significantly improve mechanical, thermal and electrical properties. Apart from these improvements, such nanofillers also offer structural damage sensing ability to materials. Structural health monitoring (SHM) is a type of a Non-destructive Evaluation (NDE) technique that essentially involves the strategic embedding of conductive filler into a structure to allow continuous and remote monitoring for damage, deformation and failure. SHM technology is applied increasingly for research and industrial purposes as a potential tool for quality assurance. However, many of the developed and available NDE technologies are complex, expensive and require significant calibration with the passage of time. Nanostructured carbon embedded systems have proven to be more sensitive towards structural damage. The current talk focusses on the development of a novel method for assessing structural damage by analysing change in the electrical conductivities of ceramic and polymer nanocomposites filled with different types of carbon nanofillers (including carbon black).

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Zeolites: Support material and stabilizing agent for silver nanoparticles

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The aim of this study is to compare the photochemical synthesis of silver nanoparticles upon natural zeolite clinoptilolite or by using PVP as stabilizing agent. On the one hand silver nitrate solution was mixed with different concentrations of PVP and the pH was adjusted to 6, 9 and 10.5. The obtained solution was exposed to the light from OSRAM Vitalux lamp (300 W and 230 V) for 1, 2 or 3 hours under continuous stirring. On the other hand clinoptilolite was suspended in silver nitrate solution. The mixture was exposed to the light from OSRAM Vitalux lamp (300 W and 230 V) for 1, 2 or 3 hours under continuous stirring. It was found that the mass ratio PVP/AgNO₃ of 1 gave AgNPs with needle-like shape (18-170 nm width and 120-1100 nm length). AgNPs became spherical with the increase of the amount of PVP in the solution. The mass ratio PVP/AgNO₃ of 10 with the pH of 10.5 was required to get spherical AgNPs that ranged between 4.42 and 75.54 nm after 3 hours of light exposure. While the exposure to the light of the mixture of clinoptilolite and AgNO₃ solution gave mono-dispersed spherical AgNPs that ranged between 2.99-6.75 nm after 3 hours of light exposure without adjusting the pH.

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Waste to Want: Polymer Nanocomposites using Nanoclays Extracted FROM Oil Based Drilling Mud Waste

Urenna V. Ekeh-Adegbotolu*

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Due to the European Union (EU) waste frame work directive (WFD), legislations have been endorsed in EU member states such as United Kingdom for the Recycling of wastes with a vision to prevent and reduce landfilling of waste. Spent oil based drilling mud (drilling fluid) is a waste from the Oil and Gas industry with great potentials for recycling after appropriate clean-up and treatment processes. This research is the novel application of nanoclays extracted from spent oil based mud (drilling fluid) clean-up as nanofiller in the manufacture of nanocomposite materials. Research and initial experiments have been undertaken which investigate the suitability of Polypropylene and Polyamide 6 as potential polymers of interest. SEM and EDAX were used to ascertain morphological and elemental characteristics of the nanofiller. DSC has been used to ascertain the glass transition temperature of the polymer. The challenges faced and future work are also discussed.

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**Effect of matrix alloy and influence of Silicon Carbide particle on hardness
and compressive strength of aluminium alloy composites**

N.Ramados^{1*}, A.Elaya Perumal², and K.Pazhanivel¹

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This article presents an effect of matrix alloy and influence of SiC particle on the hardness and compressive strength of aluminium alloys (Grade 1100), composites was examined under varying temperatures and weight percentage. The results revealed that the hardness and compressive strength of the composite was noted to be significantly higher than that of the alloy and is suppressed further due to addition of SiC particles for specified temperatures. The experimental procedures was performed using a brinell hardness testing machine for conducting hardness testing and compression testing machine to carry out compressive test. The results indicate that the high strength and hardness aluminium alloys composite could be considered as an excellent material where high strength and wear resistance components are prime importance especially designing for structural applications in aerospace and general engineering sectors.

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Flow ability and Mechanical properties of PC/copolyester Blends

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Polycarbonate (PC) is one of the most widely used engineering plastic with growing applications in automotive, electronics and electrical housing due to its high impact strength and clarity. However, the poor chemical resistance and processing limits its applications. This work produced new generics of PC and polyethylene terephthalate glycol (PETG) by blending on a twin screw extruder to enhance the chemical resistance and process ability of PC. Additionally, the blend still maintains transparency. The change of process ability were detected by melt flow index(MFI). It was found that the presence of PETG can significantly increase flow ability of the blends. Mechanical properties (Tensile properties and Izod impact strength) of the blend were investigated. Finally, the optimized composition of PC/PETG will be tested on chemical resistance.

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Partially miscible blend of Polycarbonate/copolyester BlendsHathaikarn Manuspiya^{1*}, DuengdeanChaiyong²¹ *The Petroleum and Petrochemical college, Chulalongkorn University, Bangkok, Thailand*

The effect of blending between glycol-modified poly(1,4-cyclohexylene dimethylene terephthalate) (PCTG) and polycarbonate (PC) matrix on mechanical properties, physical properties and chemical resistance were investigated. The PC/PCTG blend is expected for transparency. The blends of PC and PCTG were prepared in different ratios using a twin screw extruder and fabricated into standard specimen using an injection molding technique. A blend formed with those two polymers exhibits good chemical resistance as well as good heat and impact resistance. The blends of PC and PCTG were prepared in different ratios using the twin screw extruder and fabricated into standard specimens using the injection molding. The miscibility of these blends was evaluated by Tg measured from dynamic mechanical thermal analysis (DMA). Single Tg of partially miscible blend was found at PCTG content. Partially miscible blend offered improvement in impact strength and processability compared to those of pure PC.

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Finite Element Modelling of Woven-roving GFRP Tubes under Torsional Fatigue

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Woven-roving composites are among the most important materials used in today's modern industries. Their high specific strength and corrosion resistance, as well as their flexibility to be tailored to the end product, make them an attractive material for different applications, especially for aerospace and automotive applications [1]. Even though fibre-reinforced polymers (FRP) are widely used in a tubular form (for example, drive shafts); not much attention was paid to them in the available literature. Most of the available literature focused on understanding the mechanical behaviour of flat FRP samples, especially when it comes to fatigue loading. In addition, the use of finite element modelling (FEM) has been really limited. Moreover, the majority of the work studied unidirectional rather than woven-roving FRP.

The current study focuses on modelling the fatigue behaviour of woven-roving glass fibre-reinforced polymer (GFRP) tubes under torsional moments, using FEM. The commercial FE software ABAQUS was used to model woven-roving GFRP thin tubes, made of two plies and having two fibre orientation; either $[\pm 45]$ or $[0, 90]$. This work is an extension to the experimental work done by one of the authors, which was presented in [2], in order to understand failure mechanisms as well as progressive damage contributing to the samples failure. The multi-continuum theory (MCT), available in ABAQUS, is used to model material failure. MCT is known to efficiently extract average constituent stresses and strains from composite stress and strain, and applying the appropriate physics in order to predict composite fatigue response. Fatigue failure was examined under different negative stress ratios, and good agreement has been found with the experimental results. Failure mechanisms have been identified, based on the applied stress level, to be either matrix cracking or a mix of fibre failure and matrix cracking.

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Effect of matrix alloy and influence of Silicon Carbide particle on hardness and compressive strength of aluminium alloy composites

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This article presents an effect of matrix alloy and influence of SiC particle on the hardness and compressive strength of aluminium alloys (Grade 1100), composites was examined under varying temperatures and weight percentage. The results revealed that the hardness and compressive strength of the composite was noted to be significantly higher than that of the alloy and is suppressed further due to addition of SiC particles for specified temperatures. The experimental procedures was performed using a brinell hardness testing machine for conducting hardness testing and compression testing machine to carry out compressive test. The results indicate that the high strength and hardness aluminium alloys composite could be considered as an excellent material where high strength and wear resistance components are prime importance especially designing for structural applications in aerospace and general engineering sectors.

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**Preparation and some properties of natural rubber/thermally reduced
graphite oxide nanocomposites by latex technology**

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The latex technology is an innovative alternative for the preparation of composites of natural rubber (NR) and thermally reduced graphite oxide (TRGO). To achieve an improvement of material properties is indispensable to prepare stable suspensions of TRGO. In this work the influence of two surfactants, such as sodium dodecyl sulfate (SDS), as ionic, and Pluronic F 127 as non-ionic surfactant, on the dispersion of TRGO in NR latex and the mechanical and physical properties of the composites were studied. The results showed that the SDS surfactant is ideal for preparing latex NR/TRGO nanocomposite. An optimum dispersion of the nanoparticles in the polymer matrix was achieved in the presence of SDS, as reflected in a considerable improvement of the physical and mechanical properties of the material. Thus, the nanocomposites with 3 phr of TRGO exhibited an improvement of nearly 400% in the resistance to deformation and high network percolation electrical conductivity values around 10⁻⁶ S/cm above the static limit.

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**Synthesis and characterisation of hybrid core-shell (inorganic/organic)
nanostructured materials and their effect of millable polyurethane
nanocomposites**

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The hybrid core-shell nanostructures materials have been successfully synthesis. The organic polymer shell was successfully coated on inorganic particles by ultrasonically assisted miniemulsion polymerisation technique. The size and shape of synthesized hybrid nanoparticles were confirmed using X-ray diffraction (XRD) and transmission electron microscopy (TEM), which was found to be ~80-95 nm in diameter with spherical shape. Millable polyurethane (MPU) rubber nanocomposites were prepared with hybrid particles as a filler (0.5-2.5 wt % loading) using two-roll mill and molded on compression molding machine. Dicumyl peroxide was used as a curing agent. Mechanical property and abrasion resistance were determined using universal testing machine (UTM) and abrasion resistance tester, respectively. Physical (hardness and swelling index) and thermal (flammability and stability) properties were also studied on shore A hardness tester, flammability tester and thermo gravimetric analyzer (TGA), respectively. The extent of dispersion of filler particels in MPU matrix was studied using scanning electron microscope (SEM) and atomic force microscope (AFM). MPU nanocomposites shows improved mechanical, physical and thermal properties compared to pristine MPU composite. This dramatic improvement in properties was due to very small grain size of filler particles, which facilitate uniform dispersion of nanoparticles within the chains of MPU rubber. This improvement in properties were up to 2 wt % and decreases subsequently (2.5 wt %) due to agglomeration, filler particles starts to behave like an ordinary filler at higher wt % loading.

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Preparation and characterization of composite nanofoams based on cellulose/nanoclay

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Quality preservation of Perishable products depends on a complex combination of both their physical and chemical characteristics and the external environment. Temperature variations during storage and distribution stages is one of the main extrinsic factors affecting the quality of perishable products. Usually, the limited thermal insulation of plastic foams, that are extensively employed in packaging, do not provide a good protection. Nanofoams with pore sizes in the range of nanometers can provide double the insulation performance due to appear a Knudsen effect .In this case, the molecules of the gas do not transmit the heat properly and they become less thermal conductive. The addition of small amount of nanoparticles can reduce cell size of the foam and can improve the characteristics of polymer. Cellulose, is one of the best candidates for food packaging due to its characteristics such as renewability, safety, biocompatibility and biodegradability nature. In recent years, some new non-toxic cellulose solvents have been discovered, such as sodium hydroxide solution at cold temperature, that can supply the possibilities of utilization of cellulosic materials.

In this work we presented an extensive study of the preparation and properties of new nanoporous cellulose foams prepared from cellulose/MMT composites, via dissolution/regeneration route and drying using lyophilization in a freeze drier. Density, porosity and morphology of composite nanofoams were investigated. The approaches developed for aerogels and foams were applied to analysis nanofoams mechanical properties. Young modulus, compressive yield strength and absorption energy were obtained and studied as a function of nanofoam density. More over water vapour permeability and oxygen permeability were investigated according to ASTM standard and thermal conductivity was measured according to ISO 8301.

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Novel blends and blend-nanocomposites based on in-situ synthesized thermoplastic polyurethane-urea and nitrile butadiene rubber

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The blending of conventional polymers is an energy and cost effective route to obtain new materials with a useful combination of performance characteristics not available in individual polymers. In contrast to the high temperature melt-and solvent-blending methods, the reactive-blending of thermoplastic polyurethane-urea (PUU) with nitrile butadiene rubber (NBR) is realized in this work. The PUU was synthesized in-situ from its precursors during blending with NBR in an internal mixer to get a new kind of PUU/NBR blends. The in-situ synthesis of PUU was confirmed by the structural characterization of blends via the Fourier transform infrared (FTIR) spectroscopy and Proton nuclear magnetic resonance (¹H NMR) spectroscopy. Importantly, the ¹H NMR spectroscopic analysis shows about 90% conversion of the precursor (chain extender) to an in-situ synthesized PUU during reactive blending. Blends up to 30/70 (PUU/NBR) weight ratio were prepared, structurally characterized and compounded with curatives on a two-roll mixing mill in order to crosslink the rubber phase. The blend vulcanizates showed remarkable improvement in stress-strain behaviour, hardness, tear strength, abrasion loss and dynamic-mechanical behaviour. The preparation of blend-nanocomposites was realized by adding separately the precipitated silica and carbon black in a 30/70 blend immediately after reactive blending in an internal mixer. A detailed structural and morphological characterization of the blends and blend-nanocomposites was followed by the dynamic-mechanical analysis, differential scanning calorimetry, X-ray analysis and transmission electron microscopy. Such blends and blend nano-composites can find cost-effective utilization in areas requiring high damping characteristics, strength, tear and abrasion resistance like bumpers, industrial wheels, belting, pump impellers etc.

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Tensile behavior of silica nanofiber-reinforced Nylon 6

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Silica fillers have been used widely in the reinforcement of polymers. Commonly, silica fillers are obtained as particles, nanoparticles or drawn fibers. In this work, we employed silica nanofibers obtained via electrospinning as reinforcement in silica nanofiber-reinforced Nylon 6 composite. Silica nanofibers were prepared through in-situ sol-gel reaction using tetraethyl orthosilicate (TEOS), ethanol, hydrochloric acid (HCl) and deionized water; followed by electrospinning and calcinations at 800° C. The obtained fibers were then mixed with Nylon 6 in an injection molding machine to produce silica nanofiber-reinforced Nylon 6 samples. The composite samples with various fiber weight fractions of 0, 2.5, and 5 wt% were mechanically tested. The results showed that tensile strength and tensile modulus increased with weight fraction of silica fibers.

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**Characterisation of Physicochemical Properties of Engineering
Thermoplastic Nanocomposites**

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Recent research into advanced lightweight composite materials has led to the emergence of nano-fillers in polymer and organic composites, which has attracted considerable investment in both research and the commercial marketplace. Despite the many advantages introduced, knowledge on how the nanocomposites will perform over their entire life cycle is still limited. With a focus on fracture toughness, this research project is to look at the property-structure relationship and alterations of the nanocomposites during simulated life cycle scenarios. The overarching aim being to develop and increase the life of nanocomposite materials considering integrity, durability and reparability. Additionally, the research project is part of the European Commission funded SIRENA Life project. The overall SIRENA life project investigates the simulation of the release of nanomaterials from consumer products for environmental exposure assessment. The objective of this research project is to demonstrate and validate a methodology to simulate unintended nanoparticle release from nanocomposites during drilling. From this, the nano-particles emission during drilling on alternative nanocomposites will be evaluated.

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MgO and Ti-based Whiskers Prepared by Vapor Deposition

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Different MgO and Ti-based whiskers. of nanometric thickness (50-500 nm), grew on the alumina crucible or directly on the source surface, on orthogonal or radial directions.

The shape and distribution of MgO whiskers strongly depend on the distance from the evaporation source, while Ti-based whiskers grew on the source surface, probably due to a liquid-solid growing mechanism rather than a vapor-(liquid)-solid one.

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Analyzing sliding wear behavior of Aluminium-B4C nano particles and Aluminium- B4C(nearing nano) composite under dry conditions

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The effect of B4C(nano) and B4C(nearing nano 800 mesh) particles reinforcement on tribological properties of Al-based nano composite tested using pin-on-disc wear tester at room temperature under dry sliding conditions at different specific loads for different sliding distances as per ASTM G99 standards. Hardness measurement and scanning electron microscopy were used for morphological characterization and investigation of worn surfaces and wear debris. Al- B4C(nano) has more wear resistance , sufficient co-efficient of friction and lesser in weight when compared with B4C(nearing nano 800 mesh).Taguchi analysis carried out for wear rate and co efficient of friction.

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Thermodynamical interpretations and experimental studies on the formation of amorphous boron powders via CVD method using various H₂ flow rates

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Boron exhibits the properties of high melting point, high chemical resistance, high hardness, high strength and low density. These superior properties enable to use it in several high-tech usage areas from electronics to nuclear industry. Moreover, it is also used in metallurgical industry especially in high temperature applications. The most common production method for preparing high-purity boron is the gas phase reduction of boron halides or boron hydrides by hydrogen on a hot substrate.

In this study, amorphous boron powders were produced by chemical vapor deposition (CVD) method at 700°C by using BCl₃-H₂ gas mixtures. BCl₃/H₂ molar ratios of 1/4, 1/6, 1/8 and 1/10 were conducted during experiments in order to examine the effect of H₂ flow rates on the microstructure and production efficiency of boron powders. Ar was used as a carrier gas and the molar ratio of H₂ to Ar was kept constant at 1:1. Thermodynamical interpretation of BCl₃-H₂ system for different H₂ flow rates were performed using FactSage thermochemical software.

Exhaust gases were analyzed using a Fourier Transform Infrared Spectroscope (FTIR). X-ray diffraction technique (XRD), stereomicroscope (SM) and scanning electron microscope (SEM) analyses were utilized for the characterization of the final products. Densities of the final products were measured by using a gas pycnometer. The purities of the final products were determined by titration method after lime fusion. The properties of final products and the properties of commercial ones were compared with each other. Micron-scale amorphous boron powders with a purity of 99.91 % were obtained after 1 h experiment at 700°C with a BCl₃/H₂ molar ratio of 1/10.

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Tribological Studies on Silicon carbide nano particles and Silicon carbide nano particles with MoS₂ reinforcements of Al-Based nano Composite

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The effect of Silicon carbide nano particles and Silicon carbide nano particles with MoS₂ reinforcements on tribological properties of Al-based nano composite was tested using pin-on-disc wear tester at room temperature under dry sliding conditions at different specific loads for different sliding distances. Hardness measurement and scanning electron microscope were used for morphological characterization and investigation of worn surfaces and wear debris. Al-SiC(nano) with MoS₂ composite has more wear resistance, sufficient co-efficient of friction and lesser in weight when compared with Al-SiC(nano).

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A novel technique for development of Aluminum alloy matrix/TiB₂/Al₂O₃ hybrid surface nanocomposite by friction stir processing

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Compared with non reinforced aluminum, the aluminum matrix composites reinforced by ceramic phase present high elastic modulus, High wear resistance, High specific strength, Better corrosion resistance at high temperatures and fracture behaviors, which make them as reliable material for aerospace and automotive application. However, their low ductility and softness, which are inherent properties of non formable reinforcing materials, have limited their applications. Typically, the Material life cycles depend highly on the surface behaviors. Therefore, an optimal situation is to improve the surface layer through reinforcing them by ceramic powders; while the bulk material retains the original compositions with a ductile behavior. In this research work, Friction stir processing (FSP) was used to fabricate Aluminum Alloy Matrix/TiB₂/Al₂O₃ hybrid nanocomposites for surface applications. The effects of some process parameters such as: probe profile, rotational speed and the number of FSP passes on nanoparticle distribution were studied. The improved distributions of nanoparticles were obtained after each FSP pass. By increasing the rotational speed, a better nanoparticle distribution was obtained.

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Novel ZnAl₂O₄:SiO₂ Nano-composites for High Temperature RefractoryGunjan Sukul¹ and P.V. Balaramakrishna¹*Larsen & Toubro Ltd, Hydrocarbon-IC, 3rd Floor R&D Bldg., Gate No. 1, Saki Vihar Road, Powai (W) Mumbai 400072 India*

High Temperature properties in nanocomposites have received significant attention in recent years due to its potential as an efficient refractory material. Nanoenabled spinel refractory products are finding widespread application owing to their enhanced temperature withstanding limits coupled with excellent abrasion resistance. Several synthesis techniques have been employed to develop these spinel nanopowders. Sol-Gel synthesis provides lower processing temperatures, control over purity, composition and easy introduction of doping elements. In this work an in-situ sol-gel route was adopted for preparation of novel nanocrystalline ZnAl₂O₄ dispersed in silica matrix. The gels of composition 5%ZnO–6%Al₂O₃–89%SiO₂ were developed by using tetraethyl ortho silicate, zinc nitrate, aluminium nitrate and ethyl alcohol as precursors. The transparent gels were converted to xero gel and subsequently to crystalline phase by controlled heat treatment. The structure and thermal behavior of these nanopowders was studied by utilizing various characterization techniques. Differential Scanning Calorimetry and Thermo Gravimetric Analysis were performed on the xero gel in inert argon atmosphere indicating the crystallization of spinel ZnAl₂O₄ and formation of oxide network. X-ray diffraction spectra were studied for samples heat treated at different temperatures in the range of 800 deg C to 1200 deg C confirming the formation of crystalline ZnAl₂O₄ phase. Fourier Transfer Infrared spectra was recorded to understand the mechanism of development of glass from xero gel and the various bond-formations during the transformation. The morphology and crystallite size of nanocrystals were observed by Atomic Force Microscopy (AFM). The crystallite size measured by AFM was in the range 23 – 28 nm and the mean size calculated using Scherrer's equation was 29 nm. This approach may enable rapid and cost-efficient manufacturing of bulk refractory nanocomposites for supporting the industrial demands of stringent continuous processes with higher availability.

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Reduced Graphene Oxide Based Functional Nanocomposite Vapour Sensors for Human Health Monitoring

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Since the survival of cancer patients depends on early detection of tumour cells, developing technologies applicable for rapid detection of carcinoma is a challenge for the researchers. Breath testing has emerged as a non-invasive technique for anticipated diagnosis of lung cancer, as the breath extract of lung cancer patients are found to exhibit variations of composition of volatile organic compounds (VOC) between healthy and ill patients. Clearly, the invention of a fast, reliable, economic and portable technique is highly required before breath testing becomes a clinical reality. Nanomaterial based sensor arrays can fulfill all these requirements and can form a solid foundation for identification of disease related VOC patterns in exhaled breath. In the present study, a novel chemo-resistive vapour sensor, comprising of functionalized β cyclodextrin-reduced graphene oxide hybrid transducer has been developed. This hybrid functional material can exploit the combined benefits of high specific surface and good electrical conductivity of graphene as well as host-guest inclusion complex formation ability and variable selective chemical modification of β cyclodextrin. The key goal of this work is, to tune the molecular selectivity of β cyclodextrin modified graphene based sensors, in order to construct an electronic nose with effective discrimination of targeted lung cancer biomarkers.

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Static and Dynamic Strain Monitoring of Advanced Polymer Composites by Carbon Nanotube Based Smart Sensors

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Polymer composites are developing faster than ever in the transportation field due to the strong demand for materials with high performance/weight ratio. Nevertheless, one of the brakes for this development is the lack of predictability of their damage under severe conditions such as crash or fatigue. Nanotechnology has brought about new prospects to monitor composites' health in order to anticipate their dramatic destruction and thus to improve their reliability. In case of glass fibre reinforced plastics (GFRP) it is possible to structure a conductive network by percolating carbon nanotubes (CNT) in the polymer matrix that can be used to sense crack initiation and propagation. Sensing skins about 0.5-1.5 μm thick made of 40 nanolayers of conductive polymer nanocomposites (CPC) were sprayed layer by layer (sLbL) directly on a glass textile structuring a 3D carbon nanotubes network. Different strategies of piezo-resistive sensing in GFRP are compared in terms of efficiency to follow mechanical solicitations and damages in both elastic and plastic domains. The electrical response of the smart CPC sensor to the accumulated damage combined with the acoustic emission (AE) technique and microscopy are utilized to sense damage initiation and propagation in laminated composites.

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Cable Type Three-Dimensional Cotton Thread Based Conductive Nanotextile for LPG Sensing at Room Temperature

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With many useful features like flexibility, lightweight, and fold-ability, wearable electronic components have rapidly been developed over the last decade and have already revealed many smart designs with applications. In order to achieve wearable displays, sensing devices, embedded vital signs monitoring devices, and portable power devices, a light weight and wearable power storage device is necessary. Recently, cable-type devices, a new concept of device architecture, which can maximize the mechanical flexibility and provide the breakthrough necessary in wearable electronics, have been developed and applied in the field of energy conversion, storage and sensing.

Generally, in order to fabricate cable-type device, a linear shaped electrode material is necessary. Cotton thread is a flexible and porous material composed of multiple individual weaving cotton fibrils, which are made of multiple cotton micro fibrils bundled together. The poly-D glucose chains based micro fibrils have a strong adsorption capacity for water and other polar solvents. It has also been reported that single walled carbon nanotubes (SWCNTs) have strong van der Waals interactions with this kind of poly-D glucose chains based micro fibrils. Therefore, SWCNTs can be coated on the surface of a cotton thread via its simple immersion in a SWCNTs solution. This can make cotton thread highly conductive without affecting its shape. Such hierarchical network creates complicated surface morphology, high porosity and high conductivity, which meet the requirements for an ideal sensing platform. The porous structure permits high mass loading of active materials which could further increase the energy storage and sensing capability. Especially, macroscopic linear shape and excellent mechanical flexibility of such material are particularly valuable for cable-type devices.

In this work, we report a novel sensor based on three-dimensional PAni/gamma-Fe₂O₃/CNT-cotton thread multi-grade nano structures prepared via a facile and reproducible three-step process. At first, we coated SWCNTs on porous cotton threads. The SWCNT coating makes these threads highly conductive. And then, PAni/gamma-Fe₂O₃ film were simply

grown on SWCNT coated cotton threads via electrochemical deposition process. Polyaniline/gamma ferric oxide based nanocomposites films exhibited excellent sensing ability toward LPG at room temperature. The films were studied for their response to LPG at different concentrations and maximum response was obtained for PAni/gamma-Fe₂O₃ (3 wt%) nanocomposites for 100-250 ppm LPG. The nano scale morphology of the composites provided a large surface area for the adsorption of gas molecules, thus enhancing the gas sensitivity. The sensing mechanism pertains to a change in the depletion region of the p–n junction formed between PAni and gamma-Fe₂O₃ as a result of electronic charge transfer between the gas molecules and the sensor. When functionalized cotton threads are used as electrodes and pristine cotton textile are used as separators, new cable-type sensor become available, which will significantly facilitate the developments of wearable electronics.

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Dielectric and Piezoelectric Behavior of Silver Nanoparticle filled in Bacterial Cellulose/Poly(Vinylidene Fluoride) Blend

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Poly(vinylidene fluoride) has been widely used as actuator, transducer and mechanical sensor in touch screen due to its high dielectric and piezoelectric properties. However, there are several restrictions; petrochemical-based material and high thermal expansion coefficient. According to this reason, poly(vinylidene fluoride) was incorporated with bacterial cellulose to lower the thermal expansion coefficient. The results showed that higher amount of bacterial cellulose can also slightly increase the thermal stability of the blends. In addition, bacterial cellulose can enhance both the dielectric constant and dissipation factor, but made the blends less transparency. In advance, to enhance the dielectric and piezoelectric properties of the blend, silver nanoparticle was introduced to bacterial cellulose structure prior to film fabrication. Finally, physical, thermal, mechanical, dielectric, and piezoelectric properties of the composites will be evaluated to obtain the optimized composition between those three parameters suitable for touch screen applications.

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Advanced Nanostructured coatings

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There is considerable interest and significant need for surface treatments that are variously described as anti-graffiti/easy-clean/anti-fouling or hydrophobic/oleophobic. These treatments ultimately generate a low energy surface irrespective of which description is used.

The chemistry and physics that enable high levels of water repellence and perhaps also oil repellence is relatively well understood. Natural analogues, such as the Lotus leaf, figure 1, provide for attractive images to enable engaging dissemination material on self-cleaning, whilst also enabling the role of surface chemistry and structural hierarchies to be explored.



Figure1. The lotus effect - water droplets on hydrophobe lotus leaf

The most widely known easy clean coatings are the fluoropolymers, but these are now under legislative pressure due to environmental considerations. In many applications the cost of not using anti-fouling coatings treatments is considerable but accepted. However there is an emerging market of new coating families to provide easy clean surfaces. These are commercially available technologies and some are used

successfully, although many of these offerings are still relatively niche and have yet to achieve broader industrial adoption and acceptance.

This talk will illustrate how the performance of anti-fouling coatings is related to their chemistry and physics at the nano-scale and the macro-scale. It will also cover the methods by which these coatings are fabricated and deposited and provide some guidance as to why widespread industrial adoption is challenging. The relative merits of a number of coatings will be discussed together with an assessment of the barriers to the future growth of low energy coatings.

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Electrodeposition of Nano-Aluminium Coatings from Aromatic Cation Based Ionic Liquids

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The present paper discuss the electrodeposition of nanometals like aluminium from different imidazolium based chloroaluminate ionic liquids: $\text{AlCl}_3/\text{l-ethyl-3-methyl-imidazolium chloride}$ ($\text{AlCl}_3/[\text{EMIm}]\text{Cl}$), $\text{AlCl}_3/\text{l-benzyl-3-methyl-imidazolium chloride}$ ($\text{AlCl}_3/[\text{BzMIm}]\text{Cl}$) and $\text{AlCl}_3/\text{l,3-dibenzyl-imidazolium chloride}$ ($\text{AlCl}_3/[\text{DBzIm}]\text{Cl}$) ionic liquids, respectively. This research aims to achieve this goal by investigating the aluminium coatings on gold substrate and study the effect of changing the ionic liquids, like. e.g. changing the organic cation on the properties of the resulting Al-coatings. It was found that the particle size of the Al-deposits was significantly reduced from the micrometer regime down to the nanometer regime when only changing the substituents of the imidazolium cations from EMIm to DBzIm, respectively. This means; the more the aromatic rings in the cation, the finer the particle size is. Whereas, the thickness and the adhesion of the Al-deposits were decreased with the presence of the aromatic rings.

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Effect of a gelatin-based edible coating containing cellulose nanocrystals (CNC) on the quality and nutrient retention of fresh strawberries during storage

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Strawberry is a non-climacteric fruit with a very short postharvest shelf-life. Loss of quality in this fruit is mostly due to its relatively high metabolic activity and sensitivity to fungal decay, mainly grey mold (*Botrytis cinerea*). In this study, the ability of gelatin coatings containing cellulose nanocrystals (CNC) to extend the shelf-life of strawberry fruit (*Fragaria ananassa*) over 8 days were studied. The filmogenic solution was obtained by the hydration of 5 g of gelatin (GEL) in 100 mL of distilled water containing different amounts of CNC dispersion (10 mg CNC/g of GEL or 50 mg of CNC/g of GEL) for 1 hour at room temperature. After this period, the solution was heated to 70 °C and maintained at this temperature for 10 minutes. The plasticizer (glycerol) (10g/100g of the GEL) was then added with constant, gentle stirring in order to avoid forming air bubbles and also to avoid gelatin denaturation until complete homogenization. Strawberries (purchased at the local market) were immersed in the filmogenic solution for 1 minute and after coated were dried at 15 °C by 24 hours. The strawberries were then kept under refrigeration and characterized in terms of their properties (weight loss, ascorbic acid content, titratable acidity, water content). The results have shown that samples covered with GEL/CNC had a significant improvement in its shelf-life. For instance, for the control sample (without coating) the weight loss after 8 days of storage was around 65%, while covered samples loss in the range of 31-36%. Edible coating was also effective in the retention of ascorbic acid (AA) in the strawberries, while control sample presented a fast decay in the AA content, covered samples showed a slow decay in the AA concentration. Moreover, the use of GEL/CNC edible coating had an antimicrobial effect in the fruits.

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Synthesis of a High Silicon Content Material and its use as Raw Material for New Insulating Paint & Material for the Construction Industry

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This project is a European collaborative FP7 project that aims to develop a novel, sustainable and affordable technology to produce a nanostructured thermal insulating coating to improve thermal efficiency in new and retrofit buildings.

This paper will detail the development of a 60% silicon content of precursor, the synthesis of a robust aerogel material and the formulation of a new insulating paint and plaster for the construction industry.

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Nanocharacterization of Titanium Nitride Thin Films Obtained by Reactive Magnetron Sputtering

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Titanium nitride thin films are used in applications such as tribological layers for cutting tools, coating of some medical devices (scalpel blades, prosthesis, implants etc.), sensors, electrodes for bioelectronics, microelectronics, diffusion barrier, bio-micro-electromechanical systems (Bio-MEMS) and so on. This work is a comparative study concerning the influence of substrate temperature on some mechanical and tribological characteristics of titanium nitride thin films. The researched thin films were obtained by reactive magnetron sputtering method. The experiments employed two kinds of substrates: a steel substrate and a silicon one. The elaboration of titanium nitride thin films was done at two temperatures. First, the obtaining was realized when the substrates were at room temperature, and second, the obtaining was realized when the substrates were previously heated at 250 °C. The elaborated samples were then investigated by atomic force microscopy in order to establish their mechanical and tribological properties. The nanohardness, roughness, friction force are some of the determined characteristics. The results marked out that the substrate which was previously heated at 250 °C led to the obtaining of more adherent titanium nitride thin films than the substrate used at room temperature.

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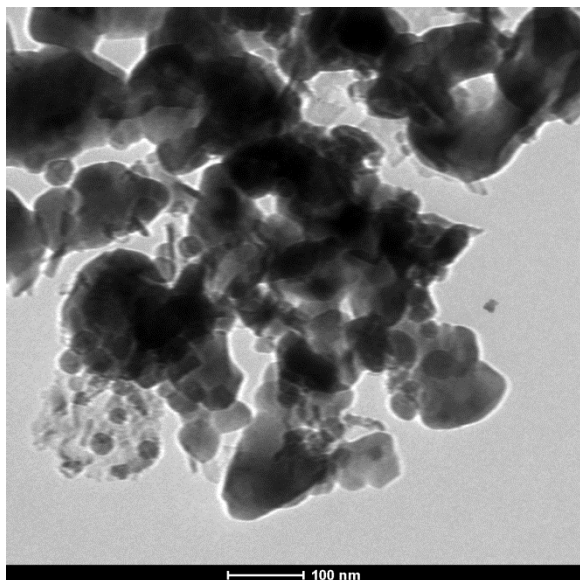
Preparation and Characterization of the NiCrAlY Nanopowder for depositing Thermal Sprayed Nanocrystalline Coatings

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There is a great movement in the application of nanosize particles in coating because it is suppose to provide a dense coating having low porosity and low stresses. Smoother surface leads better wear and erosion resistance as compared to conventional type coatings. It has been purposed by various studies that the high surface energies of the nanoparticles and the high diffusivities of the elements along the nano grain boundaries leads to the improvement in the corrosion and oxidation resistance. On the other hand thermal spray is widely used technology for developing the bulk coatings for application at high temperature power generation systems, hydro turbines and biomedical field for protection against corrosion, oxidation and wear phenomenon.

For depositing nanocrystalline coating the feedstock powder which is used during thermal spraying should be possess nanosize. Present study deals with the preparation and characterisation of the NiCrAlY nanopowders from the commercially available NiCrAlY powder by using mechanical milling. The milled powder was characterised by using FESEM/EDX, XRD and TEM studies. It has been found that the mechanical milling of the



NiCrAlY for 12 hours able to produce nanoparticles of the range 30-100nm. This nanosized powder was used as feed stock to deposit the NiCrAlY nanocrystalline coatings by using Low Velocity Oxy Fuel thermal spray technique. The coatings were then characterised by using TEM and it was found that the grain size of the coatings lies in the range 40-100nm.

Figure: TEM image of the Nanocrystalline NiCrAlY coating deposited by LVOF method.

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Silver Nanoparticles on Zinc Oxide Thin Film: An insight in Fabrication and Characterization

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In this work, a simple two-steps process has been explained to fabricate silver (Ag) nanoparticles on Zinc Oxide (ZnO) thin film followed by their characterizations. The underneath layer ZnO thin film, as an example, was also investigated how the properties change during the course of nanoparticles fabrication. ZnO thin film was sputtered on standard glass substrate followed by further sputtering of an ultrathin Ag layer. Subsequently the specimen was treated at high temperature in inert environment. A periodic observation at specific temperature intervals confirmed the formation of Ag nanoparticles on ZnO thin film. Field-emission scanning electron microscopic (FESEM) observations revealed the size distribution of as-fabricated Ag nanoparticles in the range of 50-250 nm. Elemental analysis was also confirmed by SEM-aided energy dispersion spectroscopy. The underneath layer ZnO thin film was found to go through recrystallization, stress relaxation, and grain growth during the annealing process. Further treatment to ZnO only film showed a variation in surface topology with reference to those with Ag nanoparticles on ZnO. Such a system was also analysed with finite different time domain (FDTD) analysis. A typical model was considered and FDTD simulation was carried out to understand the trend of absorption depth profile within the absorbing layer involved in plasmonics solar cell.

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Microfibrillated Cellulose Nanofibers from Eucalypt Wood: Mechanical Extraction and Application in Starch Films

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The effects of addition of eucalyptus microfibrillated cellulose nanofibers on the optical, mechanical, and microstructural properties of corn starch (plasticized with glycerol) films were studied. The microfibrillated cellulose nanofibers were obtained in a grinder by mechanical defibrillation. Starch films with 0%, 1%, 2% and 3% (by wt%) content of microfibrillated cellulose nanofiber were prepared. The starch/nanofiber films exhibited higher transmittance and lower ultraviolet absorption and reflexion. The presence of nanofibers have not showed influence in the transparency and color parameters of the plain starch films. The presence of nanofibers in the starch films increased the puncture strength. The morphology of the fracture surface of the films produced was investigated by SEM. Agglomerates of ghost granules of starch were observed on the cross section of the starch/nanofiber films. These structures are envelopes of gelatinized starch granules remaining after majority of internal starch polymers have been released. Films with 1% and 2% (by wt%) of cellulose nanofibers presented the higher rate of water vapor transmission (WVTR) compared to plain starch film and films with 3% of nanofibers. The lower WVTR for films with 3% of nanofibers is probably consequence of the closed net formed by the nanofibers into the starch film, which turn difficult the permeability of the film. The starch/nanofiber films obtained in this work presents potential to a wide range of applications such as optical instruments, flexible polymer substrates for flexible OLEDs (organic light-emitting diodes), architecture of engineered composites, agricultural uses and food packaging with antimicrobial properties.

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Preparation and Characterization of Bio-nanocomposite Films based on Zein/ Montmorillonite and determined Migration of Nanoclay from Packaging Film into Food

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Corn zein is a biopolymer which is potentially suitable for food packaging. So, in this study a montmorillonite reinforced zein nanocomposite film is prepared through solvent casting method and its structural, mechanical and barrier properties are investigated.

Based on XRD observations, solvent casting method results in a partially exfoliated structure in the nanocomposite film.

The measurements reveals that mechanical properties of the film such as young modulus and tensile strength increases as the amount of montmorillonite increases but its strain decreases. As the amount of montmorillonite increases, permeability of the film to humidity first shows decrease to the actual point and then increases.

Finally the conformity of our samples is verified based on actual regulations and European directives on biodegradable materials. The verification has done using migration tests when the films are putted into contact with food stimulants.

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Memristive Behaviour of Spin Coated Titania Thin Film

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This paper presents the memristive behaviour of spin coated titania thin films. The precursor molarity of titania thin film was varied from 0.05 to 0.4 M to study the effect of precursor molarity on the memristive behaviour of the thin films. From the observation, although the film thickness increased with the precursor molarity, the resistance ratios of the best switching loop for all samples showed no significant differences. However, it was found that the sample with less precursor molarity (device that having thinner film) required lesser time to produce the stable switching loop compared to the sample with higher precursor molarity (device that having thicker film).

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Diisopropyldiselenophosphinato-Metal Complexes – A New Class of Single Source Precursors for Deposition of Metal Selenide Thin Films and Nanoparticles

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Diisopropyldiselenophosphinato-metal complexes $[\text{Cu}_4(\text{iPr}_2\text{PSe}_2)_4]$ and $[\text{In}(\text{iPr}_2\text{PSe}_2)_3]$ were synthesized and their crystallographic structures were determined by X-ray crystallography. $\text{Cu}_2\text{-xSe}$ and In_2Se_3 thin films and nanoparticles were deposited using these complexes as single source precursors. Thin films were deposited onto glass substrates by AACVD process at temperatures ranging from 300 to 500 °C. p-XRD studies revealed deposition of $\text{Cu}_2\text{-xSe}$ (berzelianite phase) and In_2Se_3 from copper and indium precursor, respectively at all deposition temperatures. Scanning electron microscopy (SEM) showed that surface morphology and microstructure of thin films varied with deposition temperatures. $\text{Cu}_2\text{-xSe}$ and In_2Se_3 nanoparticles were grown by thermolyzing the precursors in HDA/ODE and TOP at 240 °C. As grown $\text{Cu}_2\text{-xSe}$ and In_2Se_3 nanoparticles had a mean diameter of 13.5 nm and 4.5 nm, respectively as revealed by TEM studies.

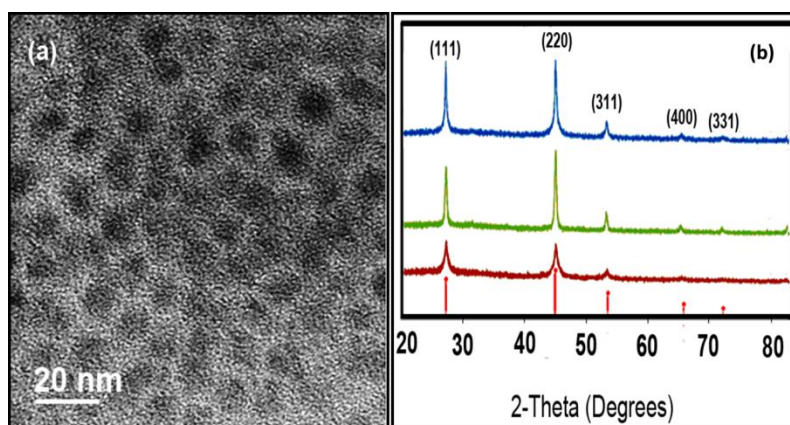


Figure 1: (a) TEM image of HDA capped $\text{Cu}_2\text{-xSe}$ nanoparticles grown from 0.3 g (0.22 mmol) of $[\text{Cu}_4(\text{iPr}_2\text{PSe}_2)_4]$ precursor at 240 °C (b) XRD patterns of cubic $\text{Cu}_2\text{-xSe}$ nanoparticles synthesized from

$[\text{Cu}_4(\text{iPr}_2\text{PSe}_2)_4]$ precursor at 240 °C indexed with the standard ICDD pattern 00-006-680 for berzelianite phase of $\text{Cu}_2\text{-xSe}$.

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Silver Nanoparticles on Zinc Oxide Thin Film: An Insight in Fabrication and Characterization

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electrons distribution with reference to those of macro-scaled counterpart. The challenge is how to fabricate these nanoparticles in cost-effective method as well as without hampering optical, electrical and topographical properties of other layers involved in device fabrication. In this study, a simple two-steps process was adopted to fabricate silver (Ag) nanoparticles on zinc oxide (ZnO) thin film followed by their topographic and optical characterizations. The underneath layer ZnO thin film, as an example, was also investigated thoroughly how the properties change during the nanoparticles fabrication. In the process, ZnO thin film was sputtered on standard glass substrate followed by further sputtering of an ultra-thin Ag layer. Subsequently the specimen was treated at high temperature in inert environment (e.g. Argon/Nitrogen). A periodic observation at specific temperature intervals confirmed the formation of Ag nanoparticles on ZnO thin film. Field-emission scanning electron microscopic (FESEM) observations revealed the size distribution of as-fabricated Ag nanoparticles in the range of 50-250 nm. Elemental analysis was also confirmed by SEM-aided energy dispersion spectroscopy. On the other hand, the underneath layer ZnO thin film was found to go through recrystallization, stress relaxation, and grain growth during the annealing process evident in X-ray diffraction measurements. Optical absorption results showed a reduction of the Urbach tail as well indicating a band gap shift of ZnO thin film. Such an attempt to fabricate Ag nanoparticles on ZnO thin film was also discussed in view of plasmonic solar cell applications.

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Effect of Annealing Temperature on the Electrical Properties of PMMA:TiO₂ as Dielectric Films using Spin Coating Deposition Technique

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Poly (methyl methacrylate):titanium dioxide (PMMA:TiO₂) nanocomposite film were deposited on glass substrate. The effect of annealing temperature on the dielectric properties of nanocomposite PMMA: TiO₂ have been investigated. The effect of annealing temperature, especially on electrical, dielectric and the morphological properties of the thin films were investigated by current-voltage (I-V) measurement, impedance spectroscopy, and FESEM. The annealing temperatures is varies from 120 oC, 140 oC, 160 oC, 180 oC and 200 oC. The electrical properties results showing when PMMA:TiO₂ nanocomposite film annealed at 120 oC produce the lowest leakage current which is 3.14×10^{-9} A/cm² measured at 5V. Meanwhile, when the annealing temperature increased, the current increased drastically from 10^{-9} to 10^{-6} A/cm² due to the perforated morphology which can be seen on the nanocomposite film. Result from the dielectric properties indicate that film annealed at 120 oC has the best relative permittivity, $\epsilon_r \sim 12$ measured at 1 kHz and the capacitance ~ 475 pF compared to other temperature. The FESEM results show that as the temperature increased, the PMMA:TiO₂ nanocomposite film started to create a phase separation between the PMMA matrix and TiO₂ nanoparticles. The surface roughnesses between 19 nm \sim 33 nm is increased due to the TiO₂ nanoparticles are attracted to each other and caused the agglomeration to occur on the thin film. Overall, when the annealing temperature increased, the electrical, dielectric and morphology properties of PMMA:TiO₂ nanocomposite film are no longer having insulating properties because of the pinhole occurred on the film and the produced poor quality films.

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Synthesis and Characterization of Boron Nitride Nanoparticle/Sulfonated polysulfone/Polyvinyl Phosphonic Acid Composite Membranes

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Hexagonal boron nitride (h-BN) particles have attracted increasing interest in the scientific community due to mechanical properties¹, chemical stability², electrical features³, thermal stability⁴ and good lubrication property⁵. Acid functional polymers such as sulfonated polysulfone and polyvinyl phosphonic acid are commonly used as proton conductive membranes in fuel cells⁶. In this work hexagonal boron nitride nanoparticles were used as inorganic fillers which increase the mechanical and thermal stabilities of the polymers. Polysulfone was sulfonated with high degree of sulfonation (140%). Polyvinyl phosphonic acid was synthesized via free radical polymerization. Hexagonal boron nitride nanoparticles were incorporated into sulfonated polysulfone/polyvinyl phosphonic acid matrices and homogeneous membranes were obtained. FT-IR and ion exchange capacity measurements verified the sulfonation of polysulfone. Thermogravimetric analysis (TGA) showed that the composite membranes are thermally stable up to 200 oC. Scanning electron microscopy (SEM) verified the homogeneous dispersion of the nanoparticles in the polymer matrix. The presence of BN nanoparticles in the matrix enhanced the thermal and mechanical stability. Maximum proton conductivity was obtained as 10⁻³ S/cm in anhydrous state.

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Nano and Macro Porous Membranes à La Carte

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Nano porous anodic alumina is a widely studied material that is used for corrosion protection of aluminum surfaces or as dielectric material in microelectronics applications. For more than 40 years porous alumina has been the subject of investigations. It exhibits a homogeneous morphology of parallel pores which grow perpendicular to the surface with a narrow distribution of diameters and interpore spacings, the size of which can easily be controlled between 10 and 400 nm. Monodomain porous alumina templates with very high aspect ratios can also be synthesized by using lithographic preparation. The combination of self-assembly and lithography allows the preparation of porous alumina templates with various configurations of pore arrangement that are not accessible by other state-of-the-art methods.

Macro porous silicon, prepared by an electrochemical process, has also gained interest in research for many applications which have a demand for mechanical and chemical stability as well as a high order of the pores. The pore diameters can differ from 700 nm up to 10 μm using lithographic pre-structuring. The standard deviation of pore diameter and interpore distance is lower than 1 %. Because of the lithographic pre-structuring technique macro porous silicon with its high ordered structure represents an ideal 2-D photonic crystal (PC) exhibiting novel properties for the propagation of infrared light within the pores.

Because of the above mentioned unique properties, nano porous alumina and macro porous silicon can be used in a wide range of applications, such as filters, as platforms for multi-functional sensors, for fuel cells, and especially as templates for the fabrication of nanometer-scale composites, such as nanotubes or nanowires by electrochemical deposition or by using polymer melts.

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Analysis of Zeolite as a Prospective Candidate for Emission Control System

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Linde Type A Zeolites are synthesized in the current study by a simple Sol-Gel technique. We found that the crystal growth was controlled by varying the hydrogel synthesis time and the annealing temperature. The resulting products at various crystallization times and temperatures are studied with X-ray powder diffraction (XRD), High resolution transmission electron microscopy (HRTEM), Scanning electron microscopy (SEM), Energy dispersive study (EDS), Thermo gravimetric Analysis (TGA). Microstructure and size in HRTEM images of the final LTA zeolite annealed at 500 degree Celsius revealed the formation of cubic structure. XRD analysis revealed the higher levels of crystallization at varying temperatures. LTA zeolites were dispersed in Poly ethylene glycol (PEG) in the ratio 1:20 and coated on porous alumina beads for the formation of membrane. The membranes revealed excellent formation of fine structure LTA zeolite membrane with uniform coating under SEM study. The membrane consisted of top layer with thickness of 1.14-2.0 μ m. Crystals in the top layer showed cubic morphology and amorphous phase was observed at grain boundary between LTA zeolite and alumina substrate.

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Efficiency Improvement of Direct Absorption Solar Collectors using Metallic Nanoparticles

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Solar thermal collectors have various applications in water heating or space conditioning systems. Due to the low efficiency of the conventional collectors, the researchers have presented some suggestions for improvement in the collector efficiency. Adding nanoparticles to the working fluid in direct absorption solar collector, which has been recently proposed by some researchers, leads to improvement in liquid thermal and optical properties such as thermal conductivity and absorption coefficient. This results certainly in collector efficiency enhancement. In this paper, radiative transfer and energy balance equations are numerically solved and the effect of different metallic nanoparticles on the collector efficiency is investigated. It was found that under similar operating conditions, the presence of Aluminum nanoparticles increases the collector efficiency by about 15% compare to a flat-plate collector. This improvement is around 7% for silver and gold nanopaticles.

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Melting of Boron-Nitride armchair nanotube

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The solid–liquid phase transition of Born-Nitride (BN) armchair nanotubes are examined by classical molecular dynamics (MD) simulation. The interatomic potential employed in our MD simulation was Tersoff many body potential. We apply external thermal energy and derive Energy-Temperature, Lindeman index-Temperature and Volume-Temperature curves for armchair nanotube. The temperature and pressure of nanotube were controlled by Nose-Hoover thermostat and Berendsen barostat, respectively. Periodic boundary condition (PBC) was applied along the axis of nanotube. The thermal properties of (6,6), (8,8), (10,10), (12,12), (14,14), (16, 16) and (18,18) BN nanotube including cohesive energy, melting temperature, isobaric heat capacity and thermal expansion coefficient were investigated within an isobaric-isothermal ensemble. Our MD results show that the melting temperature of BN armchair nanotube increase with the increase in the size of nanotubes radii, but this dependence is not linear and approach a constant value at larger radii. Inversely, the cohesive energy of BN nanotube decrease with the increase in the size of nanotube radii, but this dependence is not linear and approaches a constant value at larger radii. These results agree with the results for carbon nanotube.

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Anti-Aging Elastomer Reinforcement by Antioxidant Loaded Clay Nanotubes

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Halloysite nanotube (HNT) is an economically viable two-layered aluminosilicate with a predominantly hollow tubular structure in the submicron range. The size of halloysite particles varies within 1-1.5 μm in length and 10-15 nm of inner diameter. Due to its high aspect ratio ($L/D \sim 30$), it gives a large amount of filler-polymer interactions compared to spherical nanoparticles improving mechanical and thermal properties of the polymeric composites. Loading these tube lumens with Antioxidant RD and Antioxidant 4010NA and then doping them at 3-5 % into styrene-butadiene rubber (SBR) allows for controlled sustained release halloysite nanotube openings, increasing the amount of antioxidant used in the rubber composite. Halloysite surface hydrophobization through silane or cationic amphiphiles coating allowed for better dispersion of these clay nanotubes in rubber. Direct blending of organic acids also improved the performance of SBR/HNTs nanocomposites with. The aging resistance of SBR/HNTs was studied by oxygen adsorption and heat aging method. After aging, less decrease of mechanical properties was performed by the antioxidant loaded HNTs reinforced SBR than the HNTs reinforced SBR with adding antioxidant directly while mixing. The results indicate the antioxidant loaded HNTs not only worked as fillers but also can be used for improving aging resistant.

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Reinforcing Aluminium with carbon nano tube and Characterisation of Aluminium- Nano Composite

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Reinforcing aluminium matrix with carbon nano tube by melt stirring method is the important work of this project . Different wt. fraction of 2.5%, 3.5% and 4.5% of carbon nano tubes was added to Aluminum [1100] separately to make aluminum nano composites and its mechanical, physical and thermal properties have been investigated using tensile test, hardness test, scanning electron microscope, X-ray diffraction and coefficient of thermal expansion. The result obtained for mechanical, physical and thermal properties has been compared with pure aluminum [1100].

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Graphite to Graphene via Graphene Oxide: An Overview on Synthesis, Properties, and Applications

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There is intense interest in graphene in fields such as physics, chemistry, and materials science, among others. Interest in graphene's exceptional physical properties, chemical tunability, and potential for applications has generated thousands of publications and an accelerating pace of research, making review of such research timely.

Here is an overview of the synthesis, properties, and applications of graphene and related materials (primarily, graphite oxide and its colloidal suspensions and materials made from them), from a materials science perspective.

In this review, we discuss the most recent progress on graphene-related nanomaterials, including doped graphene and derived graphene nanoribbons, graphene oxide, graphane, fluorographene, graphyne, graphdiyne, and porous graphene, from both experimental and theoretical perspectives, and emphasize tuning their stability, electronic and magnetic properties by chemical functionalization.

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Structure-property relationships in poly(L-lactic acid) nanocomposites

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Structure-property relationships in polymer nanocomposites based on poly(L-lactic acid) (PLLA) as matrix and graphene oxide (GO), graphene oxide modified with dodecylamine (org-GO) and silica nanoparticles as filler at various compositions were investigated by a variety of experimental techniques. WAXS, AFM, TEM, Polarized Light Microscopy (PLM), and FTIR techniques were used to study structure and morphology. Thermal transitions were studied by DSC, molecular mobility by dielectric techniques (Broadband Dielectric Relaxation Spectroscopy – DRS and Thermally Stimulated Depolarization Currents – TSDC), mechanical properties by stress-strain measurements, and biodegradation by enzymatic degradation measurements. WAXD patterns confirmed the exfoliation of GO and org-GO in the respective nanocomposites. Acceleration of crystallization and increase of the degree of crystallinity were observed in these nanocomposites under both isothermal and non-isothermal conditions. In the silica nanocomposites the crystallization rate increases at 2.5wt% filler and decreases at higher filler fractions. WAXD did not reveal any additional type of polymer crystallites in the nanocomposites. The mechanical properties of PLLA were found to improve after addition of GO and org-GO, with an optimum for nanocomposites containing 1wt% nanofiller and slightly better performance of PLLA/org-GO nanocomposites, as compared to PLLA/GO nanocomposites. Biodegradation rates were enhanced in the nanocomposites. Special attention was paid to the investigation of polymer-filler interfacial interactions and their effects on the final properties of the nanocomposites. To that aim, combined DSC/TSDC/DRS measurements were employed and the results were analyzed in terms of glass transition temperature and heat capacity jump (DSC), resp. time scale and strength of the segmental relaxation (TSDC and DRS).

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Superb Electrocatalytic Activity for the Oxygen Reduction Reaction at N-doped CNT-Graphene Composite Electrodes

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An electrocatalyst for the oxygen reduction reaction (ORR) is crucial in fuel cells and vital to the development of advanced electrochemical devices such as metal-air batteries. Replacing the expensive noble metal catalysts, which still only offer limited service life, with cheap and readily available materials for ORR applications is arguably the most important issue facing these technologies. Recently, nitrogen (N) doped carbon nano-materials have shown promise as Pt-free catalysts for ORR. Herein, two kinds of N-doped carbon nanotube/graphene composites were developed: (i) N-CNT/N-RGO is synthesised from a pre-doped carbon nanotube and graphene; (ii) N-CNT-RGO is synthesised by first preparing a carbon nanotube/graphene oxide composite and then N-doping applied. X-ray photoelectron spectroscopy (XPS) reveals that although the overall nitrogen content of N-CNT-RGO (~ 8%) surpasses that of N-CNT/N-RGO (~5%), the ratio of graphitic N (nitrogen in graphene basal plane) to pyridinic N in N-CNT/N-RGO (0.87) is higher than that of N-CNT-RGO (0.64). Raman spectroscopy data also confirm the prevalence of nitrogen bonding contributions into the graphitic basal plane in N-CNT/N-RGO, which is the most efficient type of doping for ORR enhancement. Electrochemical tests showed that while the N-CNT-RGO exhibits high catalytic activity toward the ORR and favors a close four-electron pathway, the N-CNT/N-RGO operates at significantly higher current density and delivers superior electrocatalytic performance for the ORR with 100% selectivity for complete four electron reduction of oxygen in alkaline aqueous solution compared to a commercial Pt/C catalyst. Furthermore, the N-CNT/N-RGO demonstrates remarkable tolerance to methanol, thereby avoiding the crossover effect and very high stability with 93% relative current retention compared with the loss of more than 40% of the cathodic current in commercial

Pt/C under 5000 continuous cycling test. The extremely high electrocatalytic activity and durability of N-CNT-N-RGO indicate that this new catalyst has potential applications in energy storage applications.

Zero Bias Anomaly in an Individual Suspended Electrospun Nanofiber

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We report observing a double broad Kondo-like zero bias conductance peak at low temperatures in individual suspended electrospun nanofibers Poly(methyl methacrylate)-multiwalled carbon nanotubes. This anomalous behavior is suppressed at higher temperatures. We attribute this to the existence of correlated double impurity system inside the nanofiber. From the results we calculate a Kondo-like temperature for the nanofiber to be ~31.7-34K.

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Effect of the Number of Layers of Graphene on the Electrical Properties of TPU Polymers

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In this paper graphene and few layers graphene were synthesized by a modified Hummers method using flake graphite powders as the starting material. The effect of the incorporation of graphene on the electrical properties of thermoplastic polyurethane (TPU) was investigated via two processing techniques: solution blending and melt compounding. When solution blending is used for the preparation of composites, the obtained electrical conductivity is higher, even at very low loads (0,25% w/w). Moreover, the single layer graphene shows 10.000 times higher electrical conductivity than few layers graphene.

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Mechanical Properties of Individual Composite Poly(methyl-methacrylate) -Multiwalled Carbon Nanotubes Nanofibers

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Multiwalled carbon nanotubes with their superb mechanical properties are an unique filler material for polymer composites. Here, we present an investigation of mechanical properties of electrospun Poly-(methyl-methacrylate) multiwalled carbon nanotubes composite nanofibers. The method of electrospinning was used to fabricate suspended individual Poly-(methyl-methacrylate) multiwalled carbon nanotubes nanofibers. In order to reinforce the nanofibers, different high concentration of multiwalled carbon nanotubes were used. Transmission electron microscopy measurements reveal a successful filling of the nanofibers. The different types of nanofiber were deposited at SiO_x substrates. Which were previously etched, to create trenches for bend tests. Followed by fixing the nanofiber with a focus ion beam platinum deposition at the trench edges. An atomic force microscopy was used to perform the mechanical nanofiber bending tests over trenches. The results were compared with pristine Poly-(methylmethacrylate)nanofibers to nanofibers with 15 weight% and 20 weight% multiwalled carbon nanotubes composite fibers. We observed that pristine nanofibers have Young's modulus of 136 MPa, while for composite nanofibers with 15 weight% have 2.65 GPa and with 20 weight% have 6.06 GPa (at room temperature and air ambiance). This corresponds to an increase of Young's modulus of 19 fold between the pristine nanofibers and the 15 weight% of multiwalled carbon nanotubes filled nanofibers. Therefore the increase of the Young's modulus compared between the pristine and the 20 weight% MWCNT filled nanofibers corresponds to 45 fold.

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Influence of Carbon Nanotubes on the Properties of Epoxy based Composites Reinforced with a Semicrystalline Thermoplastic

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Novel ternary nanocomposites based on a thermoset (TS) system composed of triglycidyl p-aminophenol (TGAP) epoxy resin and 4,4'-diaminodiphenylsulfone (DDS) curing agent incorporating 5 wt% of a semicrystalline thermoplastic (TP), an ethylene/1-octene copolymer, and 0.5 or 1.0 wt% multi-walled carbon nanotubes (MWCNTs) have been prepared via physical blending and curing. The influence of the TP and the MWCNTs on the curing process, morphology, thermal and mechanical properties of the hybrid nanocomposites has been analyzed. Different morphologies evolved depending on the CNT content: the material with 0.5 wt% MWCNTs showed a matrix-dispersed droplet-like morphology with well-dispersed nanofiller that selectively located at the TS/TP interphase, while that with 1.0 wt% MWCNTs exhibited coarse dendritic TP areas containing agglomerated MWCNTs. Although the cure reaction was accelerated in its early stage by the nanofillers, curing occurred at a lower rate since these obstructed chain crosslinking. The nanocomposite with lower nanotube content displayed two crystallization peaks at lower temperature than that of pure TP, while a single peak appearing at similar temperature to that of TP was observed for the blend with higher nanotube loading. The highest thermal stability was found for TS/TP (5.0 wt%)/MWCNTs (0.5 wt%), due to a synergistic barrier effect of both TP and the nanofiller. Moreover, this nanocomposite displayed the best mechanical properties, with an optimal combination of stiffness, strength and toughness. However, poorer performance was found for TS/TP (5.0 wt%)/MWCNTs (1.0 wt%) due to the less effective reinforcement of the agglomerated nanotubes and the coalescence of the TP particles into large areas. Therefore, finely tuned morphologies and properties can be obtained by adjusting the nanotube content in the TS/TP blends, leading to high-performance hybrid nanocomposites suitable for structural and high-temperature applications..

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Influence of Carbon Nanotubes on Mechanical Properties and Structure of Rigid Polyurethane Foam

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Carbon nanotubes characterize with high strength, high thermal and electrical conductivity, they are resistant for high temperature action. Because of these features they suppose to be promising filler for polymer composites. However it is difficult to obtain uniformly dispersion because of tendency of nanofiller to agglomeration. Also it is well known that addition of carbon nanotubes to polymers increase their strength but impact on properties of rigid foam is less known.

In this work we would like to verify influence of carbon nanotubes on mechanical properties of rigid polyurethane foam.

Multi wall carbon nanotubes with high purity 95% supplied by Nanocyl and Polyurethane system supplied by BASF were used. Nanotubes were dispersed in polyol by using three roll milling. To this matrix isocyanate was added mixed with mechanical stirrer and put in to mold. For foam structure and dispersion control scanning electron microscopy observations was carrying out. Mechanical properties were measured by tensile and bending test. Tensile and bending strength were evaluated.

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Spinning, Structure and Properties Of PP/Carbon Black And PP/CNT Composite Fibres

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Conductive carbon black pigments (CBP), carbon nanotubes (CNT) and short carbon microfibers (CMF) are the most often used as conductive dispersed phase in the polymers and polymer fibres. The main drawback of these usually high filled and oriented materials is their insufficient processing in spinning and strong decrease of their mechanical properties. In this paper, the effect of the compatibiliser-dispersant on rheological properties and melt spinning of the polypropylene (PP) composites, containing CBP and CNT (nano)filers, was investigated. Further, the supermolecular structure and selected properties of composite fibres (mechanical, electrical, barrier, thermal), were studied. The microscopic observation revealed the significant effect of the compatibiliser on morphology of the PP/CNT fibres. Selected mechanical properties of the fibres were improved mainly at lower content of CNT. Electrical properties of the composite fibres were measured using two methods: standard four contact method (FCM) and resistivity of the linear textile method (RLT). The results revealed, that percolation threshold for PP/CBP composite fibres was situated within the concentration of 15 - 20 wt%, what is two-four times higher than for PP/CNT fibres. The electrical conductivity of PP composites has been reduced at lower cross-section of the measured samples and strongly decreased with orientation of the fibres.

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Parametric Study of Carbon Nanotubes Grown Directly on Stainless Steel Substrate

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Large competition all over the world for the synthesis of cheap, scalable, and high quality carbon nanotubes (CNTs) due to its extraordinary mechanical, thermal, and electrical properties, which provide a wide range of potential applications. In this study, CNTs were synthesized by plasma-enhanced chemical vapour deposition (PECVD) directly on a stainless steel (SS-316) substrate without the addition of external metal catalyst resulting in reduction in cost. Mixtures of CH₄/H₂ feeding gases were used for the growth of CNTs. The different parameters affecting carbon nanotube growth were undertaken by varying temperature, inductive power, time, gas mixture ratio, gas mixture pressure, and surface roughness. The deposited samples were observed by scanning electron microscopy (SEM) and 3D laser scanning microscope (3D-LSM). Variation of CNTs length, diameter and density were observed from one sample to another depending on certain parameter. Characterization was carried out by fourier transform infrared spectroscopy (FTIR) to obtain the quality of the synthesized CNTs by evaluation of functional groups, Raman spectroscopy to check the nature of CNTs, and X-ray diffractometer (XRD) to obtain some information on the interlayer spacing, the structural strain and the impurities for the grown CNTs.

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Mechanical, Thermal and Electrical Properties of LDPE Filled With Carbon Nanotubes

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Carbon nanotubes (CNTs) reveal outstanding electrical and mechanical properties in addition to nanometer scale diameter and high aspect ratio, consequently, make it an ideal reinforcing agent for high strength polymer composites. Low density polyethylene (LDPE)/CNT nanocomposites were prepared via melt compounding. Mechanical and electrical properties of (LDPE)/CNT nanocomposites with different CNT contents were studied in this research. Thermal and electrical conductivities in LDPE/CNT nanocomposites were studied based on CNT content, LDPE crystallinity degree, and LDPE alignment. It was also found that thermal conductivity depends on the percolating CNT network.

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Nanofibrillated Cellulose: Sustainable Nanoparticles with outstanding reinforcing potential

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The extraction of nanosized fibrils from cellulose fibres represents, undoubtedly, the most breakthroughs in cellulose-based materials during the past two decades. This is not only evident in academic articles, but it is also manifested by the increasing number of nanocellulose patents that are published every year. Unlike the synthetic nanoparticles, nanocellulose is completely renewable, lightweight material with density around 1.5 g/cm³, inexpensive to produce and safer to handle compared to synthetic nanoparticles.

Currently, cellulose nanocrystals (CNC) and nanofibrillated cellulose (NFC) constituted the two main families of nanosized cellulose. The former is extracted from fibres after a complete dissolution of the non-crystalline fractions, while the latter results from the application of high shearing forces of disintegration leading to a high degree of fibrillation, which yields highly interconnected fibrils. Applications of nanocellulosics include reinforcement of composite materials, tissue engineering scaffolds, moistening masks for cosmetic applications, filtration media, thickening agents, rheology modifiers, adsorbents, paper reinforcement, etc.

In this presentation, an overview on the preparation, characterization and applications of nanofibrillated will be reviewed. The emphasis will be put on the activity we have carried out on this topic during the last decade and the approach adopted to reduce the energy demand during the preparation of NFC. Some aspects regarding the use of NFC as nanofiller or strength additive for paper will be also presented..

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New Products made with Lignocellulosic Nanofibers from Brazilian Amazon Forest

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The biodiversity of the Amazon forest is undoubtedly rich; hence there is considerable variety of plant fibers regarding their morphological, chemical and structural properties. The legal exploration of the Brazilian Amazon is based on sustainable management techniques, but the generation of a relevant amount of plant wastes still can't be avoided. The correct destination of such materials is a challenge that Brazilian companies have to face. In this context, the National Council of Science and Technology (CNPq) promoted the creation of investigation nets on sustainability of Brazilian agribusiness. The Brazilian Net on Lignocellulosic Composites and Nanocomposites was then created, with partnership between several national and international research institutions. Until the moment, the results showed that Amazon plant fibers that are discarded as residues have great potential to nanofiber production. Nanopapers with considerable high mechanical and physical strength, proper opacity and great crystalline index were produced by using a clean and simple mechanical method. Those materials are candidates to several uses such as packaging, substrates transparent conductive films, gas barrier films, solar cells and e-papers.

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Fibrillated Cellulose and Block Copolymers as a Modifiers of Unsaturated Polyester Nanocomposites

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Novel nanostructured unsaturated polyester (UP) resin-based thermosets, modified with poly(ethylene oxide-b-propylene oxide-b-ethylene oxide) block copolymer (BCP) and sisal microfibrillated cellulose (MFC), were developed and analyzed. UP/BCP mixtures behavior in nonreactive and reactive mixtures were studied through differential scanning calorimetric (DSC) and dynamical mechanical analysis (DMA). By considering the miscibility of the each block before and after curing, using DSC and dynamic light scattering (DLS) was determined that the formation of the nanostructured matrices followed a self-assembly mechanism. MFC prepared mainly by mechanical treatment using a high pressure homogeneizer was employed as reinforcement for nanostructured thermoset. The BCP was used as nanostructuring agent of matrix and also as dispersing agent for MFC. UP system modified with both 1 wt % MFC and 5 wt % of BCP led to design optically transparent nanostructured thermosetting materials. The final morphologies and the transparency of the designed thermosets were investigated using atomic force microscopy (AFM) and ultraviolet-visible spectroscopy (UV-vis), respectively. Finally, the mechanical properties by means of flexural modulus (E) and critical stress intensity factor (K_{Ic}) were studied showing that modifications successfully reduced the brittleness of the UP matrix increasing the toughness and allowed to maintain the flexural modulus in the UP/EPE20/MFC designed materials.

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Principle and Equipment of Melt Differential Electrospinning Preparing Ultrafine Fiber

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Two methods preparing polymer ultrafine fiber have been developed: solution electrospinning and melt electrospinning, among which, solution electrospinning is much simpler to realize in lab or industry. More than 100 institutions have made endeavors to research it and more than 30 thousand papers have been published. However, its industrialization was restricted in some extent because of existence of toxic solvent and low strength caused by small pores. Solventless melt electrospinning is environment friendly, but high melt viscosity, thick fiber diameter, low yield and complex equipment lead to less research on it. Aiming to solving the shortage of traditional needle nozzle equipment, we first proposed a melt differential electrospinning method preparing ultrafine fiber, through which fiber smaller than 1micrometer can be produced and a yield of 10-20g/h can be achieved by a needleless nozzle. Further more, principle and equipment of melt differential electrospinning are introduced.

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Biocomposite Films Based on Nanoclay in Ordered “Brick And Mortar” Structures

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Nacre is a widely studied biological composite with interesting mechanical properties¹. Nacre-mimetic composites have for this reason been prepared in several studies⁷⁻⁹. Although the materials are very interesting in structure and properties, the preparation procedures are quite complex and time-consuming. The use of papermaking-like processing methods to make brick and mortar composites of high volume fraction is therefore attractive^{5-7, 10-12}. These methods have the potential also in large-scale industrial processing. In the present work, montmorillonite clay (MTM) was combined with a high molar mass xyloglucan polysaccharide matrix (XG)^{8,9}. The XG was adsorbed to the MTM surface so that XG-coated colloidal particles were obtained in water suspension. This made it possible to use a papermaking type of filtration process without loss of polymer. The resulting biocomposite showed an ordered brick and mortar structure at the nanoscale. The MTM/XG interface was analyzed at the molecular scale, using molecular dynamics simulation. Chemical modification of the XG was also used to improve interfacial adhesion in the presence of water molecules. Resulting materials showed a clay volume fraction of around 45%. The Young's modulus was as high as 30 GPa with a tensile strength of 150MPa. With a weaker interface, the strength was 100MPa, the Young's modulus 14GPa and the strain to failure about 1%, with apparent yielding and a more tough behavior. These nanocomposite films are truly multifunctional with excellent oxygen barrier properties (also at high relative

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humidity), potential for optical transparency, and good fire retardant characteristics. The potential of these materials include replacement of aluminium barrier films in packaging applications and surface layers in fire retardant surface layers in high-performance composites.

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Mechanical and Moisture Barrier Properties of Titanium Dioxide Nanoparticles and Halloysite Nanotubes Reinforced Polylactic Acid (PLA)

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A hybrid material is a material that includes two moieties blended on the molecular scale. Commonly one of these compounds is inorganic and the other one organic in nature. Polylactic acid (PLA) has been larger used in biomedical field due to its low toxicity and biodegradability. The aim of this study was to produce PLA nanocomposites, by extrusion, containing Halloysite nanotubes (HNT) and/or titanium dioxide (TiO₂) nanoparticles, with different morphologies, nanotubes and spheres. The nanocomposites were prepared with a mono extruder with a screw diameter of 14 mm and an L/D ration of 30. The film samples were obtained by compression molded in a press with a temperature profile of 235 ± 5°C for 2.5 min, after pressing, films were cooled up to room temperature. The mechanical tests were performed according to ASTM D882-09 and the water vapor permeability was measured according to ASTM E-96, in triplicate. The tensile properties indicated that the modulus was improved with increased TiO₂ content up to 1g/100g PLA. The Young's modulus (YM) of the PLA was increased from 3047 MPa to 3222 MPa with the addition of 1g TiO₂/100g PLA. The TS of films increases with the TiO₂ content. In both cases, the YM and TS are achieved at the 1% content of TiO₂ and is due to the reinforcing effect of nanoparticles. The WVP of samples was increased by increasing the nanofiller content. It should be expected that an increase of nanofiller content would decrease the mass transfer of water molecules throughout the samples due to the increase in the way water molecules will have to cross to permeate the material. However, this was not observed. Therefore, this result can be explained considering the molecular structure of both fillers, which contain several hydroxyl groups in the surface, making the end material more hydrophilic.

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Predictive Multiscale Modeling of Nanocellulose Based Materials and Systems

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Cellulose Nanocrystals (CNC) is a renewable biodegradable biopolymer with outstanding mechanical properties made from highly abundant natural source, and therefore is very attractive as reinforcing additive to replace petroleum-based plastics in biocomposite materials, foams, and gels. Large-scale applications of CNC are currently limited due to its low solubility in non-polar organic solvents used in existing polymerization technologies. The solvation properties of CNC can be improved by chemical modification of its surface. Development of effective surface modifications has been rather slow because extensive chemical modifications destabilize the hydrogen bonding network of cellulose and deteriorate the mechanical properties of CNC. We employ predictive multiscale theory, modeling, and simulation to gain a fundamental insight into the effect of CNC surface modifications on hydrogen bonding, CNC crystallinity, solvation thermodynamics, and CNC compatibilization with the existing polymerization technologies, so as to rationally design green nanomaterials with improved solubility in non-polar solvents, controlled liquid crystal ordering and optimized extrusion properties^{1,2}. An essential part of this multiscale modeling approach is the statistical-mechanical, 3D-RISM-KH molecular theory of solvation², coupled with quantum mechanics³, molecular mechanics⁴, and multistep molecular dynamics simulation⁵. The 3D-RISM-KH theory provides predictive modeling of both polar and non-polar solvents, solvent mixtures, and electrolyte solutions in a wide range of concentrations and thermodynamic states. It properly accounts for effective interactions in solution such as steric effects, hydrophobicity and hydrophilicity, hydrogen bonding, salt bridges, buffer, co-solvent, and successfully predicts solvation effects and processes in bulk liquids, solvation layers at solid surface, and in pockets and other inner spaces of macromolecules and supramolecular assemblies⁶. This methodology enables rational design of CNC-based bionanocomposite materials and systems. Furthermore, the 3D-RISM-KH based multiscale

modeling addresses the effect of hemicellulose and lignin composition on nanoscale forces that control cell wall strength towards overcoming plant biomass recalcitrance⁷. It reveals molecular forces maintaining the cell wall structure and provides directions for genetic modulation of plants and pretreatment design to render biomass more amenable to processing. We envision integrated biomass valorization based on extracting and decomposing the noncellulosic components to low molecular weight chemicals and utilizing the cellulose microfibrils to make CNC. This is an important alternative to approaches of full conversion of lignocellulose to biofuels that face challenges arising from the deleterious impact of cellulose crystallinity on enzymatic processing.

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Numerical Modeling of FRPC reinforced with Metal Oxide Nanoparticles using Abaqus

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Continuous-fiber/epoxy-matrix laminated composites are a key structural material, due to their good properties (high specific strength and stiffness, lower density, high fatigue endurance, high damping and low thermal coefficient) and have found expanded in many applications. Civil construction industry have been found in the fibre-reinforced polymer composites (FRPC) a strengthening material to solve many problems associated with the reinforcement and deterioration of infrastructures. In general, the most used matrix in this type of laminate is the epoxy resins (EP), which is a thermoset polymer matrix that, after cure, displays some excellent mechanical, thermal, electrical and chemical properties. However, EP show poor resistance to crack initiation and propagation and is brittle. So, in recent years, a considerable amount of research has been carried out to improve the fracture resistance (toughness and brittleness) of epoxy resins. The most common studied technique consist in the incorporation of metal oxide nanoparticles into the polymer matrix to significantly affect the properties of the matrix, even with low filler volume fractions. This lead to lighter weight materials because most of the mechanical properties are enhanced. However, it still not exist reliable models to describe the inclusion of the interface elements, to model the delaminations at the interfaces between different oriented layers with, eventually, cracked matrix between layers, as well as to to help to define and implement appropriate criteria according the interaction between the delamination and the matrix cracking in composites considering the nanocomposites as reinforcement.

In this paper, an attempt is made to review and highlight some recent findings and also some trends to show future directions and opportunities to develop a new numerical model using the ABAQUS software, based on the implementation of a new methodology, which considers the interaction between the matrix cracking and the delamination.

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Structure, Entanglements and Dynamics of Polymer Nanocomposites containing Spherical Nanoparticles

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The addition of spherical particles with dimensions on the nanometer scale to a polymer can result in materials with significantly improved properties. Even though polymer nanocomposites have been extensively investigated, many basic questions regarding the molecular origin of their properties are not solved. Understanding the polymer dynamics is particularly important when designing fabrication methods for nanocomposites. Recently, polymer tracer in PS/ silica nanocomposites [1] and PMMA/silica nanocomposites [2] has been measured. The polymer diffusion is observed to be significantly slower than that predicted by the Maxwell model.

The structure, entanglements (topological constraints), and dynamics of polymer nanocomposites containing spherical nanoparticles is investigated by means of molecular simulations for both unentangled and entangled polymers. In particular, we performed stochastic molecular dynamics simulations on a bead-spring model of polymer melts and bare spherical nanoparticles in order to identify the influence of nanoparticle size, loading, and polymer-nanoparticle interactions on the overall polymer structure, nanoparticle dynamics and free volume, below and above the percolation threshold. We found that the overall polymer conformation, as characterized by the radius of gyration is perturbed due to the presence of the nanoparticles for polymer radius of gyration greater than the nanoparticle radius. Moreover, we determine the primitive path [3] by using topological algorithms [4] and observe that the entanglement length decreases with the addition of nanoparticles, and is altered by the nanoparticle size and polymer-nanoparticle interactions. Small nanoparticles are the the most effective at reinforcing the polymer matrix.

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Solar thermal collectors are applicable both in the water heating and space conditioning systems. Due to the low efficiency of the conventional collectors (about 50-60%), a number of suggestions have been proposed for the improvement of the collector efficiency. A recently proposed suggestion, adding nanoparticles to the working fluid in direct absorption solar collector, leads to improvement in the working fluid thermal and optical properties such as thermal conductivity and absorption coefficient. The use of such nanofluids can enhance the efficiency of the solar collectors. In this paper this idea is further investigated numerically by adding carbon nanohorns to the water as the working fluid of solar collectors.

The radiative transfer and energy equations are numerically solved using the finite difference scheme. Due to the small dimensions of the collector the fluid flow is assumed to be laminar and fully-developed in the collector. Thus, a parabolic velocity profile is used for the simulations.

The results show that the collector efficiency can be increased significantly by increasing either the height of the collector and the concentration of carbon nanohorns. However, it is found that only up to a certain limit, improvement in efficiency is feasible. Finally, it is found that the efficiency of the solar collectors utilizing aqueous suspension of carbon nanohorns ($h=5\text{mm}$, 0.05 g/l SWCNH concentration) is higher than that of a conventional flat-plate collector. At the same conditions, the collector performance can be further improved by adding nanohorns in proportion to aluminium nanoparticles to the base fluid.

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Modeling of Bioresorbable Nanocomposites on the Base of Chitosan Fibers with Chitin Filler

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In recent years, the natural polysaccharides and, in particular, chitin and chitosan were used for the elaboration of biocompatible and bioresorbable nanocomposites. It has been shown experimentally that the interaction of chitosan chains with chitin nanofiller leads to additional orientations of the chitosan molecules. But the mechanism of this orientation was not quite clear. To understand the molecular mechanism of the orientation, we carried out the energy minimization and molecular dynamic simulation of systems containing of one chitosan molecule on the surface of chitin nanocrystallite using OPLS and AMBER94 forcefields. Chitin nanocrystallite in our simulation contained 16 chains of chitin (4 chains in each of the 4 layers) consisting of 8 monomers. The initial conformation of chitin chains in nanocrystal were taken from the crystal structure of α -chitin. Chitosan chain in this simulation also consisted of eight monomers and have a length close to the size of the chitin nanocrystallite. To study the effect of the orientation of chitosan chains by chitin nanocrystallites we used different initial orientation angles (from 0 to 180 °) of chitosan chains relatively the chitin chains in chitin nanocrystal, where the angle of 0 ° corresponds to the orientation of the chitosan chain parallel to chitin chains in the nanocrystallite, and the angle of 180 ° - antiparallel . We obtained that the parallel (and, to a lesser extent, the antiparallel) orientation of the chitosan chains relatively the direction of chitin chains in nanocrystallites is much more profitable than all other orientations. Thus if chitin nanocrystalites are oriented they could orient the chitosan molecules. We also have shown that this result could be explained by greater number of contacts between chitosan and neighbouring chitin molecules in the case of their mutual parallel orientation.

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Infrared Nanoscopy Applied to Microbiology and Cellular Biology

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We have developed an innovative infrared microspectroscopy technique, called AFM-IR, based on the coupling between a tunable infrared laser and an AFM (Atomic Force Microscope). This coupling allows us to perform ultra-local infrared spectroscopy and chemical mapping at the nanometer scale. The principle¹ is based on detecting the local thermal expansion of the sample, irradiated at the wavelength of its absorption bands. This expansion is detected by the AFM tip in contact mode. As the duration of expansion and relaxation of the sample is always shorter than the response time of the cantilever in contact, the excitation transmitted to the cantilever acts as an impulse function, exciting oscillations at resonant frequencies of the cantilever. The technique can create nanoscale IR absorption spectra by recording the amplitude of these oscillations as a function of wavelength and chemical maps by measuring the oscillation amplitude as a function of position. We have validated this technique by comparing the infrared spectrum of a single E.coli bacterium and the corresponding FTIR spectrum, and showing the possibility to perform chemical mapping with sub-wavelength spatial resolution (50 nm)². Later, similar outcomes have been obtained in nanophotonics (20 nm resolution)³.

Our work is now mainly focused on microbiology⁴ systems and cell imaging⁵. For example, we are now interested by the production optimization of bio-polymer (PolyHydroxyButyrate) done by a photosynthetic bacteria, Rhodobacter sphaeroides. The AFMIR technique allows us to easily detect the polymer (PHB) vesicles inside the bacterium due its specific absorption band (ester carbonyl at 1740 cm^{-1}) that is different from those of the bacterium. Similar studies are also provided on different bacteria like Streptomyces to optimize the production of bio-fuel precursor (triacylglycerols).

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Scalable High-Aspect Ratio Bio-Metallic Nanocomposites for Cellular Interactions

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We synthesized high aspect ratio composites with biological and metal components. Scanning electron microscopy (SEM) and Transmission Electron Microscopy (TEM) revealed linear morphology and smooth surface texture. SEM, TEM and light microscopy showed that composites have scalable dimensions from nano- to micro-, with diameters as low as 60 nm, lengths exceeding 150 μm , and average aspect ratio of 100. The structures are stable, remaining intact for over one year in dried form and in liquid, and did not aggregate, in contrast to metal nanoparticles such as iron and copper. Many metal nanoparticles are toxic to cells, limiting their use for biological applications. The bio-metallic composites characterized here showed lower toxicity compared to their precursor metal nanoparticles in brain tumor cell cultures. Due to these more biocompatible properties, we tested the ability of the composites to interact with cells. Zeta potential analysis indicated that composites carry a net negative charge (-24.3 ± 2.2 mV), while the starting metal nanoparticles measured (43.3 ± 2.4 mV). We labeled the composites with poly-L-lysine fluorescein isothiocyanate (PLL-FITC), which shifted the potential to 3.5 ± 2.9 mV. It was observed by fluorescence microscopy that composites smaller than cells were internalized by some cells and larger composites remained outside. Cells became fluorescent over time due to leakage of PLL-FITC from the composites which lost fluorescence over time. Higher biocompatibility, low aggregation, and ability to control size distribution of the linear composites may make them ideal vehicles to deliver drugs or other materials to cells, and may be used as a scaffolding material for cells.

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High-Aspect Ratio Bio-Metallic Nanocomposites for Cellular Interactions

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We have synthesized a high aspect ratio, linear composite that has biological and metal (nanoparticle) components. Scanning electron microscopy (SEM) and Transmission Electron Microscopy (TEM) revealed their linear morphology and smooth surface texture. SEM, TEM and light microscopy images showed that composites have scalable dimensions from nano- to micro-, with diameters as low as 60 nm, lengths exceeding 150 μm , and an average aspect ratio of 100. Once synthesized, they showed a remarkable stability, remaining intact for over one year in dried form and in liquid (water), and did not aggregate, indicating a stable charge distribution, in contrast to starting metal nanoparticles such as iron and copper. Many metal nanoparticles are toxic to cells, which limits their use for biological applications. However, the bio-metallic composites synthesized here showed lower toxicity compared to their precursor metal nanoparticles in brain tumor cell cultures. Due to these more biocompatible properties, we tested the ability of the composites to interact with cells. We determined by Zeta potential measurements that composites carry a net negative charge (-24.3 ± 2.2 mV), while the starting metal nanoparticles measured (43.3 ± 2.4 mV). We labeled the composites with a number of polymers, including poly-L-lysine fluorescein isothiocyanate (PLL-FITC), which shifted the Zeta potential to 3.5 ± 2.9 mV. It was observed by fluorescence microscopy that composites smaller than cells were internalized by some cells and larger composites remained outside. Cells became fluorescent over time due to leakage of PLL-FITC from the composites which lost fluorescence over time. Features such as higher biocompatibility, low aggregation, and ability to control size distribution of the linear composites (which we carried out by sonication) may make them an ideal vehicle to selectively deliver drugs or other materials to cells. The micro sized composites may also be used as a scaffolding material for cells.

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Admicellar polymerization of PCL-PLA on NR latex particles

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This work presented synthesis of core-shell particles of polycaprolactone-poly(lactide (PCL-PLA) copolymer on natural rubber core via admicellar polymerization. Particles size, microscope images, Thermogravimetric analysis and infrared spectra of shell components are investigated to prove existence of core-shell feature. Particles size analyzer and optical microscope images showed size of synthesized particles are larger about 3 times than natural rubber particles. The microscope images also showed transparent layer around natural rubber core that mean core-shell feature is formed. Thermogram from TGA showed only one decomposition transition closed to that of natural rubber (T_d at 351 °C) that is characteristic of core-shell structure from admicellar polymerization. Infrared spectra of extracted shell layer showed function of carbonyl group of PCL and PLA at 1737.548 cm^{-1} and 1712.478 cm^{-1} respectively, and they also showed ester linkage at 1130, 1089 and 1037 cm^{-1} . The result revealed that PCL-PLA copolymer already coated on natural rubbers core as shell.

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Stress Distribution Effects Study in the Dental Implants

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The objective of this study is to analyze numerically by the finite element method the level and distribution of stresses equivalent Von Mises induced in the bone during the chewing process simulated by dynamic forces. These stresses are evaluated in terms of the nature of the implantology, that is to say, depending on the number of implants and the distance which separate aiming to propose a new technique for dental implants. This study is to analyze the intensity of the induced stress equivalent Von Mises in the bone between the implants. This embrittlement is all the more likely that the implants are located in close neighborhood another.

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Selective Enrichment and Sensitive Detection of Candidate Disease Biomarker Using a Novel Surfactant-Coated Magnetic Nanoparticles

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In this study, novel surfactant-coated magnetic nanoparticles were synthesized and evaluated for enrichment performance towards the sensitive detection of disease biomarkers. Surfactants with phosphate ester groups (RD35A and RD66) were used as a coating to reduce aggregation and to enhance the nanoparticle dispersion. Importantly, sensitive enrichment of the target proteins using the antibody-functionalized magnetic nanoparticles (Ab@MNP) was obtained, with a five-fold increase in recovery compared to uncoated magnetic nanoparticles. Similarly, phosphopeptide enrichment using the NTA@MNP in standard samples showed that the nanoparticles could selectively enrich phosphorylated peptides.

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Covalently Linked Graphene Biocomposites for Tissue Engineering

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Synthesizing suitable materials to fabricate scaffolds is one of the most challenging areas in tissue engineering. The synthesised materials should have good processability, ideal physical properties and cellular compatibility. It has been shown that the addition of nanofillers, graphene in particular, can significantly improve or adjust the properties of the polymers to meet the specific requirements of their applications. In this work, a number of natural and synthetic biopolymers were covalently linked to graphene and the properties of the resulting composites were investigated. The biocomposites were prepared using a stable dispersion of highly reduced graphene in aqueous or anhydrous solvents. The reduced graphene sheets are stabilised in solution by a small number of peripheral charged groups which can be used to form ester or amide linkages with polymer matrices. The addition of graphene to the polymer matrices resulted in significant improvements to mechanical strength and conductivity of the biopolymers and introduced a control over the extent of swelling in hydrogel composites. In addition, fibres with varying diameters and morphologies, as well as complex scaffolds could be easily fabricated using additive fabrication approaches. In vitro cytotoxicity tests showed good biocompatibility indicating a promising material for tissue engineering applications for example as conducting substrates for the electrically stimulated growth of cells.

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Biodegradable Synthetic PLA-PEG Polymeric Nanoparticles as Anti-Tubercular Drug Carriers

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Polymer therapeutics, a technological podium in the field of nanomedicine, has emerged as one of the most propitious platforms for the efficient delivery of anti-tuberculosis agents for the treatment of tuberculosis. A series of biodegradable low molecular weight Poly (lactic acid)-co-Poly (ethylene glycol) [PLA-PEG] di block copolymers were synthesized in the present investigation. The anti-tuberculosis (anti-TB) drug (Rifampicin: RIF) loaded polymeric nanoparticles was synthesized by emulsion solvent evaporation method. The different ratio of PLA-PEG di block copolymers have been characterized by FTIR and ¹HNMR studies. The RIF loaded PLA-PEG nanoparticles have been characterized by SEM, DLS and water contact angle measurements. The average particles size of RIF loaded PLA-PEG polymeric nanoparticles is 150-200nm. The nanoparticles were found to be spherical in shape. The hydrophobicity/hydrophilicity was determined by water contact angle measurements. The hydrophilicity of the copolymer increases with increase in the ratio of PEG monomer. The in-vitro release profile of RIF loaded polymeric nanoparticles was carried out by UV-Visible spectrophotometry and the release kinetics mechanism was followed by Higuchi and Korsmeyer-Peppas model. The drug loading efficiency of the RIF loaded PLA-PEG nanoparticles is 70% which is lower when compared to that of higher ratio of PEG monomer. The in-vitro release studies show uniform and controlled release for longer time (264h).

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Synthesis, Characterization, and Antimicrobial Activity of Poly(acrylonitrile-co-methyl methacrylate) with Silver Nanoparticles

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Nanotechnology is expected to open some new aspects to fight and prevent diseases using atomic-scale tailoring of materials. The main aim of this study is to biosynthesize silver nanoparticles (AgNPs) using *Trichoderma viride* (HQ438699); the metabolite of this fungus will help either in reduction of the silver nitrate-adding active materials which will be loaded on the surface of the produced AgNPs. Poly(acrylonitrile-co-methylmethacrylate) copolymer (poly (AN-co-MMA)) was grafted with the prepared AgNPs. The poly(AN-co-MMA)/AgNPs were examined against ten different pathogenic bacterial strains, and the result was compared with another four different generic antibiotics. The produced poly(AN-co-MMA)/AgNPs showed high antibacterial activity compared with the four standard antibiotics. Moreover, the grafting of these AgNPs into the copolymer has potential application in the biomedical field.

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Development of Adhesive Electrospinning Layer Containing Ciprofloxacin/Coconut Oil used as Antibacterial Wound Dressing

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Poly(vinyl acetate) or PVAc is a non-toxic adhesive for preparing electrospun fibrous membranes by blending the antibiotic and wound healing supporter for spinning into the polyurethane (PU) film used as a substrate. PU film has many good properties such as gas permeability, thin transparent film, which can be used as antibacterial wound dressing. In this study focuses on the synergistic interaction of two components between Ciprofloxacin (CPF) and coconut oil to against the effect of CPF which will be toxic to the growth of cells. The surface morphology, drug releasing, and structure properties of mats were characterized by scanning electron microscopy (SEM), UV-vis spectroscopy, Fourier transform infrared spectroscopy (FT-IR), strength properties of tissue adhesives in T-Peel by tension loading (ASTM F2256). The antibacterial activity will be challenged to pathogenic bacteria, *Escherichia coli* and Methicillin-resistant *Staphylococcus aureus* which are the representative of gram negative and gram positive, respectively. For the cytotoxicity of cell viability, the mats will be tested with L929 cells, keratinocyte cells, and human fibroblast cells will be cultured on the wound dressing surface to determine the indirect cytotoxicity test.

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Synthesis, Characterization and Effect of Silver Nanoparticles on the Antibacterial Activity of Different Antibiotics against some Gram Positive and Gram Negative Bacteria

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Nanobiotechnology is a broad and interdisciplinary area of research and development that has been growing explosively world wide recently. Metal nanoparticles have attracted a great attention due to their unique catalytic, electronic and structural properties in addition to their therapeutic application in medicine. Silver nanoparticles have diverse applications, which include antibacterial and antifungal activity. Resistance to antimicrobial agents by pathogenic bacteria has emerged as a global threat and this problem needs to be tackle urgently. In the present work, the effect of six antibiotics viz. Ampicillin, Gentamicin, Amikacin, Cephalothin, Amoxicilin and Tetracycline alone and in combination with silver nanoparticles against three Gram positive and three Gram negative bacteria has been attempted. Silver nanoparticles were synthesized using the aqueous stem extract of *Terminalia bellerica*. The synthesized silver nanoparticles were characterized by different techniques like UV-visible spectroscopy, scanning electron microscopy (SEM), Zeta potential and Fourier Transform Infra-Red spectroscopy (FTIR). The antibacterial activity of Gentamicin, Amikacin and Tetracycline increased significantly in the presence of synthesized silver nanoparticles of *T. bellerica* against all the tested six bacterial strains. The highest effect was observed against *Listeria monocytogenes* and *Escherichia coli*. It is confirmed that these biologically synthesized nanoparticles are capable of rendering high antibacterial efficacy and thus has a great potential in the preparation of drugs used against infectious diseases.

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Green Biosynthesis of Silver Nanoparticles using *Maytenus Emarginata* Fruit Extract and its Antibacterial Activity

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Antibiotic resistance by pathogenic bacteria and fungi has been continuously increasing over the past decade; hence, there is a need for the development of new antibacterial agents. In the present scenario, silver nano particles (AgNPs) have appeared as a promising antibacterial candidate in the medical field. *Maytenus emarginata* belongs to the family Celastraceae is known as Thorny staff tree in English. It is an important tree of the Indian Desert, as it is a drought and heat resistant biomass producer, provides fodder, timber, fuel and it has also immense medicinal value. All the parts of the plant like stem, bark, leaves, roots and fruits are medicinally useful. An attempt has been made to synthesis AgNPs using *M. emarginata* fruit. Biosynthesis of AgNPs was achieved by a novel, ecofriendly, simple, pollutant free, green chemistry procedure using aqueous fruit extract of *M. emarginata* as a reducing and capping agent. Rapid formation of stable silver nanoparticles was observed on exposure of the aqueous fruit extract with solution of 1 mM silver nitrate. The successful synthesis of AgNPs formation was confirmed by various spectral analysis like UV-visible spectroscopy, scanning electron microscopy (SEM), Zeta potential and Fourier Transform Infra-Red spectroscopy (FTIR). The particle size as determined by zeta potential was 96.4 nm and zeta potential was – 24.33. The synthesized AgNPs were evaluated for their synergistic antibacterial potential against few Gram positive and Gram negative bacteria using antibiotics like Ampicillin, Gentamicin, Amikacin, Cephalothin, Amoxicilin and Tetracycline. They showed potent synergistic antibacterial activity even better than the six antibiotics studied i.e. AgNPs enhanced the antibacterial activity of antibiotics. The organisms, which were resistant to antibiotics demonstrated sensitivity to antibiotics in combination with AgNPs. It is confirmed that these AgNPs are capable of rendering a high antibacterial efficacy and hence has a great potential as effective antibacterial agent.

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Synthesis and Characterization of Silver Nanoparticles using Psidium Guajava Leaves and Assessment of their Synergistic Antibacterial Activity

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The synthesis of nanoparticles using biological systems is an expanding research area because of its potential applications in nanomedicines besides being convenient and eco-friendly. In the present work we describe the synthesis of silver nano particles (AgNPs) using leaf aqueous extract of *Psidium guajava* and its synergistic antibacterial potential. *P. guajava* L. (Myrtaceae) is a well known traditional medicinal plant used in various indigenous systems of medicine. It is widely distributed throughout India. Synthesis of stable silver nano particles was achieved by exposing aqueous leaf extract with 1mM AgNO₃. The synthesis of AgNPs was confirmed by change in the extract colour from pale yellow to black and surface plasmon resonance spectra was obtained at 440 nm. Different instrumental techniques were used to characterize the synthesized AgNPs like UV-visible spectroscopy, scanning electron microscopy, Zeta potential and Fourier Transform Infra-Red spectroscopy. The particle size as determined by zeta potential was 25.4 nm and zeta potential was 47.0. The *P. guajava* AgNPs were evaluated for their synergistic antibacterial potential against few Gram positive and Gram negative bacteria using antibiotics like Ampicillin, Gentamicin, Amikacin, Cephalothin, Amoxicilin and Tetracycline. They showed potent synergistic antibacterial activity even better than some of the antibiotics studied. The best synergistic activity was against *Listeria monocytogenes* and *Escherichia coli*. The organisms, which were resistant to antibiotics, demonstrated sensitivity to antibiotics in combination with AgNPs. The important outcome of the study is development of value added products from medicinal plants of India for biomedical and nanotechnology based industries. Thus, synthesis of nanoparticles using *P. guajava* leaf can potentially eliminate the problem of chemical agents that can have adverse effects in application, thus making nanoparticles more biocompatible. Moreover, this work provides a new method for the synthesis of silver nanoparticles that is simple, easy to perform, pollutant free and inexpensive.

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New Approach on the Catalytic Oxidation of Methanol to Formaldehyde over MoO_3 supported on Nanohydroxyapatite Catalysts

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Molybdenum oxide (20 wt. %) supported on nanohydroxyapatite mixed was prepared by impregnation method and calcinated at 400°, 500°, 600° and 700°C in static air atmosphere. The catalysts were characterized by thermogravimetry (TG), differential thermal analysis (DTA), X-ray diffraction (XRD) and nitrogen sorption measurements. The gas-phase oxidation of methanol to formaldehyde was carried out in a conventional fixed flow bed reactor. The obtained results clearly revealed that the formation of CaMoO_4 spinel nanoparticles was active and selective catalyst towards the formation of formaldehyde. The maximum yield of formaldehyde was 97% on the catalyst calcined at 400 ° C. Moreover, the yield of formaldehyde was found unaffected by increasing the calcination temperature up to 700° C.

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Biosynthesis of Silver Nano Particles using Agro Waste Trapa Natans l. Fruit Rind and its Synergistic Antibacterial Effect with Antibiotics

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The use of any part of the plant for the synthesis of nano particles is considered as a green technology as it does not involve any harmful chemicals. In the present work, an attempt has been made to synthesize silver nano particles by making use of aqueous extract of Trapa natans fruit rind, an agro waste. The fruit rind of T. natans is having great potential as antibacterial agent. Synthesis of nano particles with antibacterial properties is of great interest in the development of new pharmaceutical products especially from fruit rind because waste material which is normally thrown into the environment can be therapeutically used. The synthesis of silver nanoparticles by using aqueous extract of T. natans fruit rind is simple, efficient, eco friendly, inexpensive, safe and it does not require any sophisticated instrumentation. Characterization was done by various instrumental techniques like UV-visible spectroscopy, scanning electron microscopy (SEM), Zeta potential and Fourier Transform Infra-Red spectroscopy (FTIR). Antibacterial activity was done by Agar disc diffusion method against three Gram positive and three Gram negative bacterial of six antibiotics; Ampicillin, Gentamicin, Amikacin, Cephalothin, Amoxicilin and Tetracycline alone and in combination with silver nanoparticles. These novel silver nano particles exhibited a tremendous potential antibacterial activity against multi drug resistant Gram positive and Gram negative bacteria. FTIR spectrum indicated the presence of different functional groups in capping the nano particles. The possible mechanism leading to the formation of silve nano particles is suggested.

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Preparation of Poly (vinyl alcohol) Film Contains Quaternary Ammonium Chitosan Nanoparticles Loaded Tetracycline Used as Antibacterial Wound Dressing

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This study focuses on the preparation of poly(vinyl alcohol), (PVA) films intended for wound dressing application. The antibacterial property of a dressing is required to enhance the wound healing process. Quaternary ammonium chitosan, (QCh), which was synthesized with differing degrees of Quaternization (76 %, 62 %, 79 %), calculated from ¹H NMR, by introducing quaternary ammonium groups into the chitosan backbone exhibit excellent water solubility. QCh can be prepared into nanoparticulate systems which have the many advantages of providing targeted delivery and controlling the releasing of a drug. The nanoparticle can be prepared by an ionic gelation between polycations of QCh and polyanions of tripolyphosphate, (TPP). Tetracycline (TC) possesses a wide range of antimicrobial activity against gram-positive and gram-negative bacteria which will be loaded into the QCh nanoparticles. The success of TC loaded into the QCh nanoparticles were spherical in shape with an average diameter of 60-200 nm as observed by Scanning Electron Microscopy (SEM) and Dynamic Light Scattering (DLS). As determined by UV-vis spectrophotometry, the Encapsulation efficiency (%EE) of TC loaded into the QCh nanoparticles was about 73-91 %, when the initial TC was 2.5–12.5 mg/ml. Moreover, increasing the amounts of TC loaded into QCh led to an increase of %EE but increasing the amounts of QCh brings to a decrease of %EE. The bacterial activity of TC loaded into QCh nanoparticles will be studied by dish diffusion method and the percentage of bacterial reduction against *Escherichia coli* (Gram-negative) and *Enterococcus faecium* (Gram-positive), which showed antimicrobial activity with a clear zone about 15 mm and 7 mm, respectively. The release of TC loaded into QCh nanoparticles will be study in acetate buffer solutions (pH5.5) and in phosphate buffer solutions (pH7.4). Finally, indirect cytotoxicity evaluation will be carried out on the PVA films containing the TC loaded into QCh nanoparticles by using L929 cell and fibroblast.

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Functional Polymer - Clay Nanotube Biocomposites with Sustained Drug Release

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Natural halloysite clay nanotubes with 15 nm lumen, 50 nm external diameter, and length of ca. 1000 nm are described as inorganic reinforcing materials for polymers. Loading these aluminosilicate tubes with biomolecules (antimicrobials, proteins, DNA, drugs), and doping them into polymers allows for controlled release with new smart properties. Addition of 5-8 % halloysite synergistically increases polymer strength on 50-70 %, enhances adhesivity and adds new functions due to slow medicine release. Halloysite is available in tons and is sophisticated and novel “green” nanomaterial. It is biocompatible as demonstrated with cells and small animal experiments.

Loading halloysite with antibiotic ciprofloxacin allowed for 70 hrs release time with drastically enhanced efficiency against multidrug resistant gangrene bacteria *P. Aeruginosa*. Loading halloysite with dexamethasone and resveratrol drugs allowed for 20-30 hour release. Extended 5-20 hrs release of simple antiseptics (povidone iodine, chlorhexidine, brilliant green) from halloysite also has shown higher antimicrobial efficiency.

Halloysite tubes can encase enzymes for longer storage, higher temperature functionality while the tube's opening allows for delivery of small substrate molecules into the tube interior for biocatalysis. Loading DNA into halloysite is another perspective research direction. As functional nanoblocks, halloysite tubes may be used for building on biological cells, like formation of spore-like microbial shells providing microorganisms with additional functions.

Poly(methylmethacrylate) (PMMA) bone cement, admixed with prophylactic antibiotics (e.g. gentamicin), is widely used in hip and knee replacement surgery. There is a critical need to improve its structural integrity and to control antibiotic release. We have loaded clay nanotubes with gentamicin sulfate, and doped the cement at 5-8 wt %. Gentamicin loaded nanotubes admixed in PMMA cement provided sustained release during 300-400 hours and with enhanced release at cement cracks. The PMMA/halloysite/gentamicin composite tensile strength was significantly increased (tripled). Similar antibiotic loaded halloysite was done for calcium phosphate bone implants.

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Polyurethane / POSS Hybrid Organic-Inorganic Nanomaterials

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Among different classes of nanomaterials, hybrid organic-inorganic materials (HOIMs) are considered nowadays as potential candidates to play a major role in the development of advanced functional materials. HOIMs consist of organic and inorganic components intimately mixed, where at least one of the component domains has a dimension ranging from a few tens to several nanometers, and there are chemical bonds (covalent or ionic-covalent bonds) between the components¹¹. Interesting and unique phenomena have been found in hybrid materials in the nanometer region, such as energy dissipation, (macro)molecular mobility effects, etc. Among inorganic nanoparticles, functionalized silsesquioxanes (POSS) are unique nanobuilding blocks that can be used to create a wide variety of hybrid materials, where precise control of nanostructures and properties is required. Condensed silsesquioxanes have the general formula $(\text{RSiO}_{1.5})_{2n}$, where n is an integer and R can be a large number of substituents including hydrogen, alkyl, alkylaryl, alkenyl, phenyl, halogen and siloxy groups²⁻⁵.

In this presentation general information on HOIMs and their future perspectives will be given, illustrated by polyurethane/POSS hybrid materials synthesis and properties evaluation.

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Bi-O-S System Obtained By Mechanical Alloying and Its Microstructural Characterization

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Bi-O-S system is an interesting material for superconductor applications¹, in the last two years was synthesized by solid state methods, in this work we focused on the study of Bi-O-S system obtained by mechanical alloying. Elemental powders were mixed and mechanically processed in a low energy mill (rod mill) at room temperature and powder-grinding media ratio of 1/10. In order to avoid cross contamination, grinding media of zirconia with a cylindrical shape and two different sizes (1/2 x 1/2 in and 3/8 x 3/8 in) were used. MA process was carried out in argon atmosphere and 400 rpm of rotation velocity in order to obtain nanostructured system. Different grinding times were used such as 0, 100,200,300 and 400 h. Microstructural characterization of Bi-O-S system was carried out by X-ray diffraction (XRD) and Scanning Electron Microscopy with Energy Dispersive Spectroscopy (SEM-EDS) during mechanical alloying (MA). Crystallite size, lattice strain and lattice parameter in every stage of milling were calculated using X' Pert HighScore Plus software. The results showed at 200 h of milling time, were identified monoclinic phases and at 400 h were identified tetragonal phases² with increasing grinding time 0 to 400 h a nanostructured was found with a crystal size of 70 nm, micrographs confirm there is a clear refinement of particle according with XRD results^{3,4}.

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Polypropylene Fibers Modified with Inorganic Additives for Technical Application

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Physical modification of polypropylene (PP) fibers by inorganic additives insures more intense anchoring of PP fibers in constructional composites, what leads to expressive improve of functional of PP fibers in relation to transmission and absorption of deformation energy to form and load composites¹⁻³.

This work focuses on the preparation of PP fibers modified with untreated and treated CaCO_3 and SiO_2 for constructional composites. It is investigated the effect of inorganic additives on the thermal and mechanical properties of these fibres.

Thermal properties of PP fibres modified by CaCO_3 and SiO_2 were evaluated using DSC. Thermal characteristic (melting (T_m) and crystallization (T_c) temperatures and melting (ΔH_m) and crystallization (ΔH_c) enthalpies) depend on applied additives and conditions of preparation of PP fibres. Melting and crystallization temperatures of modified PP fibres were comparable to temperatures of pure PP fibre. However, melting and crystallization enthalpy significantly decrease at modified PP fibres.

Mechanical properties of PP and modified PP fibres were study on the basis the tenacity and the elongation at the break and Young's modulus using Instron 1112. The inorganic additives decrease their mechanical properties. The decrease of properties is not very important for their application into the constructional composites.

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Microwave-assisted synthesis of nanosized Bi₂Te₃–Bi₂Se₃–Bi₂S₃ system

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Recently, Bi₂Te₃-based nanocomposites synthesized from powder metallurgy methods have drawn much attention as a result of their better thermoelectric and mechanical properties. Bi₂Te₃-based materials are also used in low-temperature (RT-300oC) heat to electricity conversion applications, including solar to electrical generation. The primary motivation of this work is to explore some new compositions within the Bi₂Te₃–Bi₂Se₃–Bi₂S₃ system to achieve higher ZT values in the mid-temperature range. Partial substitution of tellurium in Bi₂Te₃ by selenium or sulfur was used to reduce the lattice thermal conductivity thereby raising the ZT value in n-type Bi₂Te₃-based thermoelectric materials. Bi₂Se₃ and Bi₂S₃ were much less studied as thermoelectric materials than Bi₂Te₃. Recently, was found that the application of microwave radiation greatly facilitates the use of the polyol method for the preparation of binary chalcogenides. In the polyol reaction metallic nanoparticles are produced as intermediates, resulting from the reduction of their ions. Synthesis generally proceeds at a temperature above 100°C and autogenous pressure organic solvent exceeds the pressure of the environment which is favorable for the crystallization products, also prevented effectively from oxidation and volatilization and the reaction and crystallization can be realized simultaneously. Furthermore, organic solvents may be favorable for the dispersion of non-oxide nano-crystallites and may stabilize some metastable phases. In the present work, nanoparticles and nanowires have been prepared by solvothermal microwave-assisted synthesis using Bi₂O₃, TeO₂ and L-cystein as the precursors and dimethylformamide (DMF) as the solvents and ethylene glycol as a reducing agent. The microstructures and thermoelectric properties of the synthesized powders have been characterized and the relationship with the structure has been investigated.

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Roll-to-roll Manufacturing of Polymer Nanocomposites

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The aim of this paper is to elaborate on achieving uniform dispersion of nanoparticles in polymer nanocomposites. It is widely known that achieving uniform nanoparticle dispersion in polymer nanocomposites is challenging. We discuss aspects on uniform polymer nanocomposites achieved in a roll-to-roll process with increased strength-to-weight ratio by controlling uniform 3D dispersion of nanoparticles at the nanoscale in polymer matrices by a UV-NIL roll-to-roll process and self-organization of nanoparticles by a capillarity force when printing a nanoparticle dispersion. Polymer nanocomposite granules are produced by cutting as-produced substrates to pieces. The uniform 3D-array polymer nanocomposites is likely to open up new possibilities for polymer nanocomposite manufacturing for e.g. high efficiency wind-mill rotor blades.

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Nanocomposite Membranes Based on Sulfonated Polysulfone and bifunctional nanotitania for Proton Exchange Membrane Fuel Cells

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Proton conducting nano-composite membranes were prepared via ternary mixtures comprising sulfated nanotitania (TS), sulfonated polysulfone (SPSU) and nitrilotri(methyl phosphonic acid) (NMPA). The surface morphology and homogeneity of the composite membranes were searched by scanning electron microscopy (SEM). FT-IR showed the existence of ionic interaction between sulfonic acid units of SPSU/TS and phosphonic acid units of NMPA. The spectroscopic measurements and water uptake studies confirmed the complexation between SPSU/TS and NMPA that inhibited the exclusion of NMPA up on swelling in excess water. The TGA results verified that the membranes are thermally stable up to 270 °C. The T_g of the materials shifts to lower temperatures as nitrilotri(methyl triphosphonic acid) (NMPA) content increases as indicated by DSC results. From the methanol permeability experiments it was found that the permeability of the composite membranes is lower than that of commercial Nafion 112. The maximum proton conductivity of SPSU-TS-NMPA is 0.002 S cm⁻¹ at 150 °C. From the conductivity and spectroscopic results as well as literature data the possible proton conductivity mechanism of the membrane has been modelled.

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Nanofiller Modified Thermoplastic Composites

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The paper presents the obtaining and characterization of thermoplastic matrix composites modified with different nanofillers consisting of COOH-functionalized carbon nanotubes and quaternary ammonium salt modified montmorillonite respectively. The materials are obtained by melt extrusion followed by injection molding into specific shape specimens for mechanical testing of the samples. The materials are afterwards characterized by morpho-structural analysis and in terms of tensile and flexural resistance performance as well as thermal stability under load characteristics (heat deflection temperature). The results show positive effects concerning 4%wt modified montmorillonite based materials in terms of mechanical characteristics and thermal stability under load, in the case of carbon nanotubes better results were obtained for lower nanofiller content(2%wt).

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Preparation and Characterization of Polymeric Nanocomposites Containing Exfoliated Tungstenite at High Concentrations

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Exfoliated tungstenite (EWS2) is a graphene-like 2D nanomaterial with exceptional physical properties. In this work, the production of EWS2 at high concentration and its use for the obtainment of acrylic nanocomposites was investigated. For the first time, ultrasonication was exploited for obtaining tungstenite nanoparticles directly into an acrylic monomer (tetraethyleneglycol diacrylate) without any chemical manipulation and avoiding the recovery of the sonicated nanoparticles, hence preventing any possible restacking phenomenon. The resulting liquid dispersions were characterized by Raman, transmission electron and scanning electron microscopies, which confirmed the obtainment of exfoliated material. It was also found that EWS2 concentration depends on sonication time and WS2 concentration. Eventually, the dispersions were directly used for preparing nanocomposites containing a relatively large amount of exfoliated tungstenite. Differential scanning calorimetry and thermogravimetric analyses were performed in order to assess the effect of the presence of the exfoliated nanofiller on the thermal features of the polymer matrix: a clear improvement of the thermal and thermo-oxidative stability was observed. At variance, the effect of the exfoliated tungstenite on the glass transition temperature of the polymer matrix was negligible. Furthermore, the mechanical behavior of the obtained nanocomposites was evaluated by means of flexural and shore A hardness tests: the exfoliated nanofiller turned out to exert a strong reinforcing effect on the polymer matrix even at very low concentration.

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Influence of Experimental Parameters on the Morphology and Distribution of ZnO Nanoparticles on the Surface of Natural Cellulosic Fibers

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Hard natural fibers were used as matrix for the deposition of zinc oxide nanoparticles, using both thermal and sonochemical methods^{1,2}. Fique fibers, native to Colombia, are composed of approximately 63% of cellulose and have a heterogeneous surface with high oxygen density that facilitates metal oxide nanoparticle growth and stabilization, as has been previously demonstrated³. Fique fiber–ZnO bionanocomposites were synthesized by a co-precipitation method using ZnSO₄ as precursor, NaOH for hydroxide formation and thermal or ultrasound energy to promote Zn(OH)₂ decomposition and ZnO formation. The biocomposite was fully characterized using X-ray diffraction, X-ray fluorescence, Fourier transform infrared spectroscopy with attenuated total reflectance, field emission scanning electron microscopy and energy dispersive X-ray spectroscopy. We observed that experimental parameters such as [OH⁻]/[Zn²⁺] ratio, and heating or sonication time wield a strong influence on shape, size and surface distribution of ZnO crystals. Our results indicate that careful control of such parameters allow for selective deposition of ZnO with varied sizes and shapes such as ovals, bars and flowers.

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Structure and Mechanical Properties of PP/Organoclay Composite Fibres

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The incorporation of the organoclay into the semicrystalline polymers affects their supermolecular structure and mechanical properties. In addition, the structure of the polymer composites change significantly in deformation and orientation processes.

In this paper, the effect of uniaxial deformation of PP/organoclay composite fibers in spinning and drawing on their supermolecular structure, thermal and mechanical properties is presented. The commercial organoclays Cloisite C15A and Cloisite C30B, both based on montmorillonite (MMT) were used in experimental work as inorganic fillers. The supermolecular structure of fibers was investigated by DSC analysis and X-ray diffraction (WAXS). The DSC measurements were carried out using conventional method (CM) and constant length method (CLM) in which the fibers with constant length during measurement were assured. The average orientation of fibers has been evaluated by the sonic velocity method. Intercalation of polypropylene in the interlayer galleries of organoclay was evaluated by SAXS method. Tenacity and Young's modulus of composite fibers were evaluated and discussed with regard to their thermal properties and supermolecular structure as well as intercalation and exfoliation of (nano)filler in polymer matrix.

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The Comparison between the Properties of Ternary Nanocomposite

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The properties of the nanocomposite of polypropylene (PP)/ethylene–octene random copolymer (EOC) blend with double compatibilisers of maleated PP (PP-g-MA) and maleated EOC (EOC-g-MA) were investigated and compared with the similar nanocomposite containing block copolymer of ethylene-octene. Yield stress, tensile modulus and flexural modulus of two studied nanocomposite were relatively the same. However, the charpy impact strength of nanocomposite containing random EOC is significantly lower than that nanocomposite containing block EOC. There is no distinct difference between the XRD patterns of two nanocomposite. The rheological examinations indicated that the dispersion degree of clay in the nanocomposite containing block EOC is much better than that of random EOC. SEM results showed that random EOC form bigger dispersed domains than block EOC.

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Nanocomposites based on layered silicate materials: preparation, characterization and functional properties as a tool for sustainable agriculture

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Nanomaterials have been recently proposed as a tool to increase the sustainability of agricultural activity and to reduce its environmental impact.

The goal of this work was to prepare and characterize a novel functional material by the modification of SAz-1-montmorillonite with the polymer hexadimethrine (HEXAD) to explore its application in agriculture, i.e., as a strategy to enhance the adsorption of herbicides. Comparative preparation and characterization with the hexadecyltrimethylammonium-modified SAz-1-montmorillonite (SA-HDTMA) was also performed. The characterization was assessed by elemental analysis, XRD, FTIR, physisorption of N₂, scanning electron microscopy (SEM) and Z potential measurements. Both HEXAD and HDTMA were intercalated stoichiometrically into SAz-1, resulting in basal spacing values of 1.4 nm for hexadimethrine-polymer nanocomposite (SA-HEXAD) and 2.8 nm for SA-HDTMA. FTIR analysis indicated the interaction of the polymer by means of alkyl groups of hexadimethrine with the clay surface. These outcomes suggested that the polymer formed a horizontal monolayer exposing positive charges out of the interlayer space of SAz-1, as indicated by the positive Z potential of SA-HEXAD (+13.6 mV), which was in contrast to the negative value recorded for SA-HDTMA (-4.6 mV). Additionally, higher specific surface area was obtained for SA-HEXAD (51 m² g⁻¹) than for SA-HDTMA (11 m² g⁻¹) with N₂ adsorption isotherms typical for clay-nanomaterials. SEM micrographs showed no significant changes in the morphology of clay minerals upon treatment with the organic cations, suggesting “functional” character due to their different surface properties. Adsorption of several herbicides on SA-HEXAD and SA-HDTMA, was also investigated and related to their tunable properties. SA-HEXAD displayed high affinity for anionic herbicides, which were adsorbed on this nanoclay through ionic forces. SA-HDTMA presented greater adsorption than the original clay (SAz-1) for most of herbicides as a result of hydrophobic interactions.

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Effect of Hydrophobized Alumina Nanoparticles on the Thermal and Mechanical Properties of Styrene Butadiene Rubber

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Filling polymers with nanoparticles generally leads to changes in the relaxation behavior of the matrix molecules. Varying the size or chemical nature of the filler the interactions with polymer matrix and also the properties of the composite can be controlled. It is generally thought that hydrophobic nanoparticles ensure better compatibility with olefin polymers and have positive effects on the dispersion of fillers. Using dynamic mechanical analysis (DMA) and temperature modulated calorimetry (TMDSC), we investigated the influence of different amounts of untreated and silanized (by Octadecyltrichlorosilane) alumina nanoparticles on the properties of a model rubber system (SBR). The results obtained show significant influence of the chemical nature of the nanoparticles surface on the thermal and mechanical behavior of the nanocomposites which is especially noticeable at small filler concentrations. It seems that in this case hydrophobization of the filler surface leads to an acceleration of the relaxation modes responsible for the thermal glass transition, which manifests itself by decrease in glass transition temperature. The reinforcement effect is shown by DMA for all of the nanocomposites compared to the pure SBR, although it is generally more noticeable for the systems with untreated AluC. The silanization has the unexpected influence on the elastic modulus: the systems containing hydrophobic AluC have lower elastic modulus at high filler concentrations, but present higher modulus at low filler concentrations. The TMDSC data (cp' , cp'' , Δcp), as well as DMA data (G' , G'') are used to discuss the possible effect of the organic “shell” of the surface-treated nanoparticles and the possible reduction of the polymer-polymer interactions as one cause for such behavior.

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Preparation and Characterization of Ultra-Hydrophobic Calcium Carbonate Nanoparticles

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Anionic surfactants based on fatty acids are usually used to modify the particle surface properties of calcium carbonate with the aim to enhance its dispersion and compatibility with polymer matrices. In this study sodium oleate was used for the preparation of ultra-hydrophobic calcium carbonate nanoparticles using a wet carbonation route. The effect of sodium oleate on the characteristics, crystallite size, particle size, morphology, surface potential, thermal decomposition and hydrophobicity of calcium carbonate, was investigated using X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), transmission electron microscopy (TEM), Zeta potential, thermogravimetric analysis (TGA) and water contact angle measurement (WCA). The results showed that the addition of 2 wt % sodium oleate helps in reducing the particle size from 2 μm length scalenohedral particles to 45 nm rhombohedral particles and modifying of the hydrophobic property of calcium carbonate.

Bionanocomposite Adsorbents for the Removal of Water Pollutants

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Biopolymers and clay minerals can be considered as a cheap and non-hazardous source of components for the preparation of low cost bionanocomposites that can receive application in environmental remediation. These materials have emerged in the last decade as a new group of advanced materials showing improved structural and functional properties, but also provided with the non-toxic, biocompatible and biodegradable character of the involved biopolymers^{1,2}. Layered silicates of the smectite family are the most commonly used inorganic solids in the preparation of bionanocomposites³, and silicates with microfibrillar morphology are becoming also an interesting alternative for this purpose⁴.

Among many other uses, bionanocomposites began to receive application in the last years as biosorbents for the removal of pollutants from water. Thus, this presentation will give an overview on the contribution of our research group in the development of bionanocomposite materials and their application in the removal of a wide variety of water pollutants including dyes, pesticides, lanthanides and heavy metal ions. These biosorbents were based on abundant and well-known polysaccharides like chitosan⁵ or starch⁶, and also on another recently discovered biopolymer known as sacran⁷.

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**The Immobilisation of Bimetallic Fe/Ni Nanoparticles on Cellulose-based
Electrospun Nanofibers for the Degradation of DDT in Contaminated Water**Jane Catherine Ngila^{1*}, Odwa Mapazi¹ and Philemon Matabola²¹*University of Johannesburg, Department of Applied Chemistry, P. O. Box 17011**Doornfontein 2028 South Africa*²*Mintek, South Africa*

Immobilisation of metal nanoparticles on substrates such as membranes, metal oxides and clay for application in catalytic dechlorination of organohalogenes in ground water remediation is a common practise. In the current effort, the immobilisation of bimetallic Fe/Ni nanoparticles on electrospun cellulose-based nanofibers was examined with the ultimate view to apply the materials on dechlorination studies using DDT (1,1,1-trichloro-2,2-bis(p-chlorophenyl)ethane) as a model compound. Fe/Ni bimetallic nanoparticles were anchored on oxolane-2,5-dione-functionalised cellulose nanofibers by the successive reduction of Fe(II) and Ni(II) ions from their respective solutions using NaBH₄. In the mixing method, unsupported bimetallic Fe/Ni nanoparticles prepared by chemical precipitation were mixed into electrospinning solutions of cellulose acetate and then nanofibers were generated with embedded nanoparticles. The bare, functionalised and composite nanofibers were characterised using ATR-FTIR, SEM, EDS and TEM. SEM and TEM investigations revealed successful immobilisation of the nanoparticles on the nanofiber matrices. The oxolane-2,5-dione modified nanofibers decorated with nanoparticles showed good activity towards DDT dechlorination. A dechlorination efficiency of 94.8 % was attained within a period of 4 hours.

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**Synthesis of robust flexible PVDF ultrafiltration nanostructured
membranes supported on non-woven fabrics for separation of NOM from
water**

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Water purification technologies based on nanostructured membranes are prone to fouling by natural organic matter and other biological species in water. This leads to the short lifespan of the membranes and high demand in energy than normal due to high pressure needed to pump water across the fouled membrane. In a quest to address these challenges, polyvinylidene fluoride (PVDF) membranes supported on 3 different types of non-woven fabrics (NWF) were fabricated using the phase inversion method. This enabled us to modify the active top layer of PVDF thin film while maintaining the high mechanical strength offered by the NWFs. A PVDF resin was used with N-methyl-2-pyrrolidone (NMP) as solvent. PVDF is known to have inherent hydrophobic properties, we added polyvinylpyrrolidone (PVP) in the casting solution to enhance the hydrophilicity of the membranes. N-doped carbon nanotubes were also used to enhance the mechanical properties of stand alone PVDF membranes and comparisons were made. FTIR spectroscopy, sessile drop contact angle measurements, thermo-gravimetric analysis (TGA), scanning electron microscopy (SEM), atomic force microscopy (AFM) and for mechanical strength test were used to study the membranes. The membrane flux and rejection were studied using the cross-flow membrane unit. The contact angle results revealed that the hydrophilicity of PVDF membranes became hydrophilic as the PVP concentration was increased. TGA revealed that the membranes were thermally stable up to 530 °C. The cross-sectional SEM revealed that membrane pores become enlarged when PVP has been added. AFM showed that membrane roughness became improved when PVP was added. The highest rejection of humic acid (HA) recorded for PVDF membranes supported on NWF1 was found to be 97% compared to the 95% for membranes supported on NWF2 and NWF3 fabrics respectively.

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Recent Development and Future Scenario of Nanocomposites for Waste ApplicationsAjay Mishra^{*}*Department of Applied Chemistry, University of Johannesburg Doornfontein Johannesburg
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Nanocomposites are composed of nanofillers e.g nano titania, nanosilica , carbon based nanomaterial, magnetic nanoparticles, metal nanoparticles etc reinforced into variety of matrices such as polymer matrices, metal matrices and ceramic matrices. With different combination of matrices and nano-fillers, variety of nanocomposite materials have been developed for material, biomedical and environmental applications. The growing material demand with unique and fascinating properties, nanocomposites are being extensively investigated. The present work exclusively focus on the nanocomposites used for waste management application in the area of waste water treatment. Nanocomposites have been developed as an adsorbent, photo catalyst, magnetic nanoparticle based adsorbents, super absorbent using hydrogel as matrices that have been applied for uptake of heavy metals and organics and photo catalytic degradation of organic contaminants. Some of the recent development in this area of research along with the future scenario shall be addressed in this talk.

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Water Treatment with the Aid of Cyclodextrins

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The application of supramolecular entities such as dendrimers, crown ethers and cyclodextrins in composites has resulted in tailor-made materials with enhanced performance. In this presentation I will outline some of the work our group has been involved in for water treatment that combines polymers, cyclodextrins and nanoparticles. Enhanced anti-bacterial activity, better anti-fouling performance, and good selectivity without the need for problematic elements such as silver particles were achieved. These materials are now being developed for other applications outside the water treatment sector, including the development of sensors and biosensors, for medicine, and materials to aid in biotransformations.

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**CuO/Pectin Bionanocomposite with a Remarkable Visible Light
Photoactivity, Adsorbing Power and Antimicrobial Action for Waste Water
Treatment**Amit Kumar^{1, 2*}, Susheel Kalia⁴ and Pooja Dhiman³¹*School of Chemistry, Shoolini University, Solan , Himachal Pradesh, India-173212.*²*Department of Chemistry, Himachal Pradesh University, Summer Hill Shimla, India-171005*³*Department of Physics, Himachal Pradesh University, Summer Hill Shimla, India-171005*⁴*Department of Civil, Chemical, Environmental and Materials Engineering, University of
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It is still a challenge to photocatalytically remove organic pollutants as textile dyes from wastewater owing to the relatively low efficiency of photocatalysts. Also there is need for hybrid biocompatible nanomaterials which possess efficient adsorption capacity, visible light photoactivity and antimicrobial action. A novel photocatalyst pectin/copper oxide (Pectin/CuO) nanocomposite was synthesized successfully by co-precipitation followed by encapsulation with Pectin. The present investigation describes the applicability of Pectin/CuO for removal of Congo red dye from aqueous solution. The effect of adsorption capacity of Pectin on photocatalytic activity of CuO was also studied. The photocatalytic activity of composite is also compared with that of CuO nanoparticles. The composite has an excellent antimicrobial action. The materials were characterized by Fourier transform infra red spectroscopy (FTIR), X-ray diffraction (XRD), scanning electron microscopy (SEM), transmission electron microscopy (TEM), small area electron diffraction (SAED), Photoluminescence (PL) and UV-Vis spectroscopy. The simultaneous adsorption and photocatalysis proved to be a better reaction condition for photodegradation of the dye in presence of Pectin/CuO.

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Session 3.5 & 3.6– First International Workshop of the SIRENA-LIFE Project - María Blázquez

The first international workshop of the SIRENA LIFE Project will be held within the International Conference on Structural Nanocomposites, NANOSTRUC 2014.

In its 2020 Strategy, the European Union highlights nanotechnology as one of the key emerging technologies (KETs) to promote smart and sustainable growth throughout the EU area to promote the EU as the most competitive global knowledge - based society providing prosperity and social stability for its citizens¹. Engineered nanomaterials (ENM) and in particular plastic industry utilizing them for nanocomposites manufacturing provide an important path to reach these goals. In fact, according to Freedonia², by 2025, it is expected that nanocomposites will be a \$9.5 billion market, with volumes nearing five billion pounds with applications being commercialized in a variety of industrial sectors.

Within the first international workshop of the SIRENA LIFE Project, the different applications of engineered nanomaterials (ENM) in the plastics industry are outlined; the need to develop standard protocols to characterize the release of embedded nanomaterials from composite matrixes is addressed and the actually existing regulatory void in the Nanotechnology area is evaluated.

The SIRENA LIFE Project fosters the safe and sustainable development of Nanotechnology as a KET.

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¹EU Strategy 2020

²Nanocomposites - US Industry Study with Forecasts for 2011, 2016 & 2025

Lifecycle-based Fate Analysis of Carbon Nanotubes in Automotive Supercapacitor Applications

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Carbon nanotubes are considered one of the most prominent and promising materials of nanotechnology research. As an additive they have the potential to enable or enhance various technologies due to their large surface area, superior stability and electric conductivity. Double layer capacitors, which are widely known as supercapacitors, can be considered as a bridging technology between batteries and capacitors since they employ both electrostatic and electrochemical mechanisms. In the EU project AUTOSUPERCAP, carbon nanotubes are integrated in supercapacitors to substantially increase the electrodes' surface and thus the energy density of the storage devices. Despite their excellent physical characteristics, carbon nanotubes are suspected to potentially cause adverse effects on humans and other living organisms, in particular on the respiratory system. While the hazardous potential of carbon nanotubes is not consistently assessed yet and their potential toxicological triggers are not completely understood, nanotoxicity cannot be included in environmental sustainability analysis methods, such as life cycle assessment. Nevertheless, it is possible to evaluate or estimate the particle pathways of carbon nanotubes in so-called fate analysis. Particle fate is highly depending on the production, the particles' contact with the environment during the use phase and the final product treatment at the end of life. Therefore, a lifecycle-based fate analysis approach is proposed in this study focusing on a realistic application case in automotive-grade supercapacitors. The study qualitatively evaluates where, how, to what extent and in which immission regime, carbon nanotubes might come in contact with the environment or affect humans. The study can be seen as a first step towards integration of nanotoxicity considerations in the life cycle assessment of energy storage systems.

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**Comparing Production Efforts and Efficiency Benefits of Nanomaterials
over the Life Cycle: Carbon Nanotubes in Lithium-Ion Batteries**Benedikt Zimmermann^{1*} and Marcel Weil^{1,2}¹*Karlsruhe Institute of Technology, Institute for Technology Assessment and Systems
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Life cycle assessment is a widely used comparison-tool to analyse various environmental impacts of different products. By regarding the whole product life cycle from resource production, over manufacturing and use, down to the end of life treatment, the overall environmental impacts of different life phases can be compared in a rather unbiased manner. Nanomaterials, such as carbon nanotubes, promise significant technology enhancement potential. In currently produced lithium-ion batteries carbon nanotubes could be implemented, in order to increase both the electrodes' energy- and power-density. This results in lighter battery packs, so when applied in electric vehicles the cars' energy consumption can be decreased. Furthermore, the batteries' lifetime and input-output energy efficiency might also be improved. On the other hand nanomaterial's production is considered more energy intensive than the production of traditional materials. In this study, life cycle assessment is used to compare the environmental impacts of carbon nanotube production with the benefits of integrating them in a lithium-ion traction battery. The assessment is based on the battery-application in a mid-size electric vehicle. In three different scenarios the effects of battery-weight reduction, battery lifetime improvement and battery efficiency gains are compared with a non-enhanced standard-battery. All scenarios conclude that carbon nanotubes can improve the performance of the battery and thus the car, so that repercussions from carbon nanotube production can be set off during the use phase.

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**Holistic Assessment of Cellulose Nanofibre Reinforced Composites to
Obtain Sustainable Products**

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On the example of cellulose nanofibres derived from vegetable food waste, it is shown how the use of life cycle assessment (LCA), life cycle cost analysis (LCC) and other methods can influence the development and production of a material at an early point of development in order to obtain a sustainable product. This includes identifying in which applications the material has the highest potential to be used successfully in the market by combining technical, economic and ecological criteria throughout the whole life cycle. The resulting application fields are further investigated. Up-scaling calculations from the lab production process to a theoretical industrial production process are used to perform full LCAs and LCCs and prove whether environmental and economic advantages of the material compared to existing material are possible. As a result, new LCA data for products containing cellulose nanofibres reinforced composites derived from vegetable food waste is presented and compared to glass and carbon fibre reinforced polymers (GFRP and CFRP).

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Ecological Sustainability of Façade Coating Systems containing Manufactured Nanomaterials

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Within the construction sector, nanotechnologies are expected to hold considerable potential for the development of new materials. For nano-Ag and nano-TiO₂, the paint & coating industry is one of the major users of these materials. In a project together with several companies from this industry sector, the potential environmental, health and safety (EHS) impacts of coatings containing manufactured nanomaterials (MNM) have been addressed here in a holistic and prospective manner along the complete life cycle. Potential improvement of the environmental performance of these coatings has been examined with a Life Cycle Assessment (LCA) study.

The study shows that the results – i.e. if the MNM containing paint results in a better environmental performance than a paint not containing any MNM – depend on a number of factors: the MNM has to substitute an (active) ingredient of the initial paint composition and not to be simply an additional in-gredient, the new composition has to extend the lifetime (until the next application of paint on the wall) that much that this results in a reduced consumption of paint along the life cycle of a building, and releases (especially by dumping unused paint together with the packaging) of nanoparticles have to be reduced to the lowest level possible. Only when all these boundary conditions are fulfilled, an improved environmental performance of the MNM-containing paint was shown to be possible for the paint compositions examined in this study.

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**Environmental Impacts of Multiwalled Carbon Nanotubes (MWCNT) and
Platinum in Fuel Cell Technology**Dominic Notter^{1*}, Katerina Kouravelou² and Nara Haberland³¹*Swiss Federal Laboratories for Materials Science and Technology, Ueberlandstrasse 129
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Producing energy with water as only direct emissions at tailpipe is an attractive concept behind fuel cells. The expensive platinum catalyst has plagued the design of fuel cells because the environmental and economic performance is diminished by the high platinum demand. Replacing carbon black with multiwalled carbon nanotubes (MWCNT) allows reducing the amount of platinum by enlarging the catalytic active surface. The aim of this work was to use life cycle assessment to compare the environmental performance of two Fuel Cell (FC) systems, a conventional electrocatalyst using carbon black as supporter for the platinum and an electrocatalyst using MWCNT as supporter for the platinum. Industrial data was collected for the MWCNT production (Nanothinx, Greece) and the production of the electrocatalyst, while all other components of the FC rather refer to a technically sensible option than to a specific product. Environmental impacts were evaluated with Ecoindicator 99. First results demonstrate that platinum causes most environmental impacts in a FC unit (40% all of environmental impacts), even though its mass (0.0003%) is irrelevant. The production of the MWCNT as supporter for the platinum is connected with higher environmental burden than the production of carbon black (Figure 1). However, this difference is overcompensated by far with the platinum savings which leads to an overall benefit for the FC unit with MWCNT of 40% compared to the FC with CB as supporter.

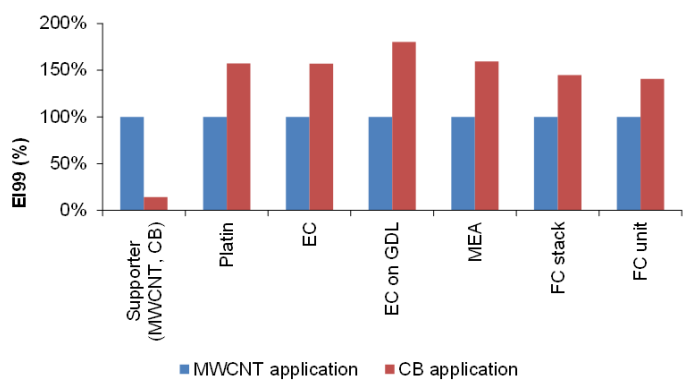


Figure 1. Mass share and the environmental impacts (EI99) for both types of fuel cells. The damage is depicted relative to the damage of the components containing MWCNT. EC (electrocatalyst); GDL (gas diffusion layer); MEA

(membrane electrode assembly).

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**Investigation of the Impacts of Selected Nanotechnology Products
Regarding their Demand for Raw Materials and Energy**

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Nanotechnology is already being used in a wide variety of applications. The conservation of resources and energy play a major role in the decision to employ nanotechnology. In the study presented here qualitative and quantitative life-cycle considerations were employed to assess the potential material and energy savings that might be achieved through the use of nanotechnology. Ten nanotechnology application fields with broad market coverage and immediate impact to either the generation of renewable energies or the use of critical resources were analyzed.

Organic photovoltaic modules (solar cells that essentially consist of organic materials) and electronically dimmable windows (electrochromic laminated glass, which can be adjusted to conform to the ambient light conditions) as two very promising nano-enabled applications were quantitatively analyzed. Eight further products including neodymium magnets were evaluated on a qualitative basis.

All assessments contain classical indicators such as energy efficiency, product carbon footprint, and resource consumption. When considering the key indicator “resource consumption”, for example, special attention was given to the evaluation of the metals and rare earths involved. In addition, pollutant aspects (exposure and toxicology) as well as other sustainability aspects (such as user benefits) were taken into account in the framework of a so-called “hot spot analysis”.

Furthermore, drivers behind the innovation as well as associated rebound effects were identified. The results highlight the importance of product specific analyses based on a life-cycle thinking approach. They are shown to be an absolute prerequisite for obtaining reliable results in the assessment and ecological optimization of nano-enabled products.

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Precautionary Design of New Nanomaterials and Nanoproducts

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The development of nanotechnology especially of next generations nanotechnology is still in an early phase of development. Here we have the collingbridge dilemma between design options and the availability of reliable impact knowledge.

As long as results from toxicological assessments are not sufficiently accurate to warrant special legal regulation of nanomaterials, their handling should be guided by a precautionary approach. There is a need for a preliminary assessment and for a rational implementation of the ‘precautionary principle’ based on sound scientific data and knowledge indicating justifiable concern.

In this contribution, the focus is placed on the developed comprehensive approach for the precautionary design of engineered nanomaterials and nanoproducts. This approach is derived from several semi-qualitative and quantitative approaches to risk assessment and to criticality of materials, and is supplemented with environmental impact categories of Life

Cycle Assessment.

Categories and aspects Data quality Source

Precautionary risk aspects

Precautionary need of humans Semi-quantit. Swiss precautionary matrix for synthetic nanomaterials¹

Precautionary need into the environment Semi-quantit. Swiss precautionary matrix for synthetic nanomaterials

Predicted environmental concentration Quantitative Probabilistic material flow analysis⁴

Precautionary need of incident Semi-quantit. German ÖI Sustainability check⁵, orientation on Swiss precautionary matrix

Ressource aspects

Criticality Semi-quantit. EU concept of criticality³

Abiotic ressource requirement Quantitative LCA methodology²

Other LCA impact categories

Energy requirement Quantitative LCA methodology

Global warming potential Quantitative LCA methodology

Human toxicity potential, but not nanospecific Quantitative LCA methodology

Eco-toxicity potential, but not nanospecific Quantitative LCA methodology

Table 1: Approach for the precautionary design of engineered nanomaterials and nanoproducts

The approach as well as first assessment results to nanomaterials (e.g. nanocellulose, MWCNT, nano TiO₂, and nano ZnO) and associated products will be presented.

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**Life Cycle Assessment of a Nano-Enhanced Supercapacitor for Automotive
Application**

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Despite technological improvements of conventional vehicles, the road transport sector remains one of the largest contributors to air emissions and energy consumption. In order to cope with these problems new drive trains and energy storage systems are being developed. Supercapacitors, also called double layer capacitors, are one of these promising energy storage systems. However, a number of problems remain, such as low energy density and high costs. The EU Project Autosupercap within the 7th Framework Program, aims at the development of next generation supercapacitors using multi walled carbon nano tubes (MWCNT) for enhancing power and energy performance while reducing weight and costs. At this stage of development it is very valuable to assess the viability of this kind of MWCNT application from a life cycle perspective, i.e. if the increased performance of the nano-enhanced supercapacitor is able to offset the additional environmental burden of the MWCNT production.

Thus, a life cycle assessment (LCA) is performed which is based on a scaled up production of supercapacitor pouch cells for automobile application including end of life considerations for the energy storage unit. A conventionally fueled vehicle as well as different cell chemistries of the supercapacitor (e.g. with and without MWCNT) shall help to identify the best technology option from an LCA point of view. Due to the lack of characterization factors for nano particles within the life cycle impact assessment methodologies, merely the known impact categories will be used in the LCA. However, a fate and subsequent hazard analysis may be done complementary to this study and subsequently incorporated into the LCA in future work. In that way an approach is presented of how to assess the environmental impact of nano materials on an automotive system level over the whole life cycle.

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**Nanotoxicity and Life Cycle Assessment: First attempt towards the
Determination of Characterization Factors for Carbon Nanotubes**

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Carbon materials, whether at macro, micro or at nanoscale, play an important role in the battery industry, as they can be used as electrodes, electrode enhancers, bipolar separators, or current collectors. When conducting a Life Cycle Assessment (LCA) of novel batteries manufacturing processes, we also need to consider the fate of potentially emitted carbon based nanomaterials. However, the knowledge generated in the last decade regarding the behavior of such materials in the environment and its toxicological effects has yet to be included in the Life Cycle Impact Assessment (LCIA) methodologies. Conventional databases of chemical products (e.g. ECHA, ECOTOX) offer little information regarding engineered nanomaterials (ENM). It is thus necessary to go one step further and compile physicochemical and toxicological data directly from scientific literature. Such studies do not only differ in their results, but also in their methodologies, and several calls have been made towards a more consistent approach that would allow us model the fate of ENM in the environment as well as their potentially harmful effects. Trying to overcome these limitations we have developed a tool based on Microsoft Excel® combining several methods for the estimation of physicochemical properties of carbon nanotubes (CNT). The information generated with this tool is combined with degradation rates and toxicological data consistent with the methods followed by the USEtox methodology. Thus, it is possible to calculate the characterization factors of CNTs and integrate them as a first proxy in future LCA of products including these ENM.

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Poster number	Authors	Title
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3	Nathalia Verissimo, Alessandra Cremasco, Rubens Caram, Rodnei Bertazzoli and Christiane Arruda	Effect of Nb and Sn on the Anatase-Rutile Transition in Biocompatible TiO ₂ Nanotubes
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